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ORNL-5138
(Third Revision of ORNL-3794)

OR TEP-II:
A FORTRAN Thermal-Ellipsoid Plot Program for Crystal Structure Illustrations

Carroll K. Johnson

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CHEMISTRY DIVISION

ORTEP-II:
A FORTRAN THERMAL-ELLIPSOID PLOT PROGRAM FOR CRYSTAL STRUCTURE ILLUSTRATIONS

Carroll K. Johnson

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CONTENTS

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Table 2.1. Summary table of all instructions

Function	1–3	4–9	10–18	19–27	28–36	37–45	46–54	55–63	64–72
Structure analysis									
Distances	0 or 2	101	ORG 1	ORG 2	TAR 1	TAR 2	D max (A)		
Dist. + ang.	0 or 2	102	ORG 1	ORG 2	TAR 1	TAR 2	D max (A)		
Princ. axes		103							
Dist. single convolute		105	ORG 1	ORG 2	TAR 1	TAR 2	D max (A)		
Dist. reiterate convolute		106	ORG 1	ORG 2	TAR 1	TAR 2	D max (A)		
Plotter control									
Initialize		201							
Advance and term.		202	X(IN)	Y(IN)					
Initialize CRT		203	XORG	YORG	IZORG				
Change CRT intensity		204	IZ-IZORG						
Plot boundary									
Dimensions		301	X(IN)	Y(IN)	VIEW(IN)	BRDR(IN)			
Title rotation		302	THETA(°)						
Retrace displace		303	X(IN)						
Atoms list									
Run add		401	FROM (1)	( ) TO (1)	FROM (2)	( ) TO (2)	FROM (3)	( ) TO (3)	. . .
Run subtract		411	FROM (1)	( ) TO (1)	FROM (2)	( ) TO (2)	FROM (3)	( ) TO (3)	. . .
Sphere add	0 or 2	402	ORG 1	ORG 2	TAR 1	TAR 2	D max (A)		
Sphere subtract	0 or 2	412	ORG 1	ORG 2	TAR 1	TAR 2	D max (A)		
Box add		403	ORG 1	ORG 2	TAR 1	TAR 2	A/2 (A)	B/2 (A)	C/2 (A)
Box subtract		413	ORG 1	ORG 2	TAR 1	TAR 2	A/2 (A)	B/2 (A)	C/2 (A)
Triclinic box add		404	ORG 1	ORG 2	TAR 1	TAR 2	A/2	B/2	C/2
Triclinic box subtract		414	ORG 1	ORG 2	TAR 1	TAR 2	A/2	B/2	C/2
Convolute add		405	ORG 1	ORG 2	TAR 1	TAR 2	D max (A)		
Convolute subtract		415	ORG 1	ORG 2	TAR 1	TAR 2	D max (A)		
Reiterate convolute add		406	ORG 1	ORG 2	TAR 1	TAR 2	D max (A)		
Reiterate convolute subt.		416	ORG 1	ORG 2	TAR 1	TAR 2	D max (A)		
Zero atoms list		410							
Cartesian system									
Definition		501	ORGN	V1A	V1B	V2A	V2B		
Rotate reference		502	Axis No.	Rotate (°)	Axis No.	Rotate (°)	. . .	. . .	. . .
Rotate working		503	Axis No.	Rotate (°)					
Translate working		504	ΔX (IN)	ΔY (IN)	ΔZ (IN)				
Origin at centroid		505							
Inertial axis system and origin at centroid		506							
Store overlap data (Also see 822, 821)	0 or 2	511	0 1 OVMRGN (IN)						

Table 2.1 (continued)

Function	1–3	4–9	10–18	19–27	28–36	37–45	46–54	55–63	64–72
Center and scale									
Explicit		601	XO (IN)	YO (IN)	SCAL1	SCAL2			
Scale only		602	XO (IN)	YO (IN)		SCAL2			
Center only		603			SCAL1	SCAL2			
Center and scale		604				SCAL2			
I.P. and I.S.[a]		611	ΔXO (IN)	ΔYO (IN)	ΔSCAL1	SCAL2			
I.P. and scale		612	ΔXO (IN)	ΔYO (IN)		SCAL2			
I.S. and center		613			ΔSCAL1	SCAL2			
Ellipsoids									
Shaded football	0 or 1	701					SYM HGT	PAR-OFF[b]	PER-OFF[c]
(Format No. 1 trailer card)			A0 (IN)	A1 (IN)	ANR (1)	ANR (2)			
Football	0 or 1	702	(same as 701)						
Open model	0 or 1	703	(same as 701)						
Boundary only	0 or 1	704	(same as 701)						
Other types	0 or 1	705	NPLANE	NDOT	NLINE	NDASH	SYM HGT	PAR-OFF[b]	PER-OFF[c]
(Format No. 1 trailer card)			A0 (IN)	A1 (IN)	ANR (1)	ANR (2)			
As above except no	0 or 1	711	(same as 701)						
printed output of	0 or 1	712	(same as 701)						
individual coordinates	0 or 1	713	(same as 701)						
	0 or 1	714	(same as 701)						
	0 or 1	715	(same as 705)						
Bonds									
Explicit	1 or 2	801	FROM (1)	TO (1)	FROM (2)	TO (2)	FROM (3)	TO (3)	. . .
(cont.)									
Implicit fancy	2	802							
(Format No. 2 trailer card)									
Implicit line	2	803							
(Format No. 2 trailer card)									
As above except		811	(same as 801)						
no printed output	2	812	(same as 802)						
	2	813	(same as 803)						
Bond overlap	1 or 2	821	FROM (1)	TO (1)	FROM (2)	TO (2)	FROM (3)	TO (3)	. . .
explicit									
Bond overlap	2	822							
implicit									
Labels									
Chem. Symb.		901	ATOM-1	(ATOM-2)	X Edge Reset	Y Edge Reset	HGT (IN)	PAR-OFF	PER-OFF
Reg. titles.	3	902	ATOM-1	(ATOM-2)	X Edge Reset	Y Edge Reset	HGT (IN)	PAR-OFF	PER-OFF
Format No. 3 title card									
Proj. Vect. title	3	903	ATOM-1	ATOM-2	X Edge Reset	Y Edge Reset	HGT (IN)	PAR-OFF	PER-OFF
Format No. 3 title card									
Vector title	3	913	ATOM-1	ATOM-2			HGT (IN)	PAR-OFF	PER-OFF
Format No. 3 title card									

Table 2.1 (continued)

Function	1–3	4–9	10–18	19–27	28–36	37–45	46–54	55–63	64–72
Proj. bond label									
(1 dec. place)		904	ATOM-1	ATOM-2	X Edge Reset	Y Edge Reset	HGT (IN)	PAR-OFF	PER-OFF
(2 dec. places)		905	(same as 904)						
(3 dec. places)		906	(same as 905)						
Bond label									
(1 dec. place)		914	ATOM-1	ATOM-2			HGT (IN)	PAR-OFF	PER-OFF
(2 dec. places)		915	(same as 914)						
(3 dec. places)		916	(same as 914)						
Centered symb. (pen up)	1	908	ATOM-1	(ATOM-2)	X Edge Reset	Y Edge Reset	HGT (IN)	PAR-OFF	PER-OFF
(pen down)	1	909	(same as 908)						
(Format No. 1 trailer card)			SYMB#						
Saved sequence									
Start		1101							
Stop		1102							
Execute		1103							
Terminate job		1							
New job follows (from title card on)		2							

---

[a] I.P. and I.S. signifies increment position and increment scale.
[b] PAR-OFF signifies parallel offset (in.).
[c] PER-OFF signifies perpendicular offset (in.).

2.2 Programming a Nonstereoscopic Illustration for OR TEP

2.2.1 General Comments on Automated Graphics. – In order to produce high quality illustrations with OR TEP, one must in general use an iterative approach; that is, the illustration must usually be computed and plotted several times before an optimal figure is produced. With each trial, as many factors as possible are optimized to give a more informative and more esthetically pleasing result. One often requires about four trials for a stereoscopic figure of an unfamiliar structure (barring blunders and plotter malfunctions).

Overlap is one of the major problems, particularly for chemical symbols and bond distance labels. If the user is not drawing stereoscopic figures, it is often better to do the lettering with a LeRoy lettering template instead of the computer. The template lettering is neater than the computer lettering, and it can be positioned much more easily. However, for stereoscopic lettering the manual procedure appears to be unsatisfactory because of the necessity for exact relative placement of the lettering on the two views to maintain good stereopsis.

The major portions of the hidden line segments of atoms and bonds that are partially or totally behind other atoms and bonds may be omitted by using the overlap-elimination features of OR TEP-II. However, there are often areas where additional manual touch-up is needed. This can be accomplished by erasing or "whiting out" the remaining unwanted line segments. Even with stereo views, the features are more effective if overlap is taken care of, especially when "opaque" ellipsoids are used.

In order to maintain generality in OR TEP, the concept of programming is applied to the problem of drawing illustrations with a plotter. This concept allows access to a series of basic building block operations which are put together by the user to "program" an illustration. The instructions used in programming OR TEP are divided into the following categories: (1) instructions used to specify preliminary graphical details, (2) instructions used to compose an illustration, (3) instructions used to draw the illustration, (4) instructions used to repeat a sequence of other instructions, and (5) termination instructions. Each instruction starts on a separate punched card and contains an identifying number and whatever parameters are needed for the particular instruction. The general role of these instructions is explained in the remaining parts of Sect. 2, and the individual instructions are described in detail in Sect. 3.3. The simplest way to construct the program is, first, to scan through the list of instructions in numerical order and pick out the relevant ones to construct the framework of the program. Then certain other instructions are placed into the framework program to furnish the remaining "bookkeeping" details.

Let us assume that the structural data cards (described in 3.2) have been prepared for a crystal structure and that we want to prepare a program to draw a single nonstereographic figure of the contents of one unit cell. We describe next the general stepwise procedure one would follow to program such an illustration.

2.2.2 Preliminary Graphical Details. – The first instruction card should be the plotter control instruction 201 (see 3.3.3.1) which will initialize the plotting package.

Next, the plot boundary instruction 301 (see 3.3.4.1) is needed to set the following parameters: (1) *X* dimension in inches for the plot boundary, (2) *Y* dimension in inches for the plot boundary, (3) viewing distance in inches for perspective projection (zero as a signal for parallel projection), and (4) border (or margin) dimension inside the boundary.

No other 200 or 300 series instructions are required for this particular hypothetical figure.

The preliminary graphical details are analogous to what a draftsman might do in setting up his drafting board in preparation for a drawing.

2.2.3 Composing the Illustration. – This step involves specifying: (1) which atoms are to be used as the figure subject, (2) the rotational orientation of the subject, and (3) the scaling and positioning of the subject relative to the drawing area. These three components of composition are implemented by the 400, 500, and 600 series instructions respectively.

For our hypothetical example, suppose we want to place the *b* crystal axis along the plotter *x* axis and the *c* axis of the crystal in the plotter *xy* plane as nearly as possible parallel to the plotter *y* axis. This setting can be accomplished with a 501 instruction (see 3.3.6.1) alone, but if additional reorientation were necessary, a 502 instruction (see 3.3.6.2) would also be used.

A triclinic box of enclosure can be described with a 404 instruction (see 3.3.5.4) to contain the desired atoms for the subject definition. The scaling and positioning of the subject to fill the drawing area may be accomplished automatically with a 604 instruction (see 3.3.7.1).

2.2.4 Drawing the Illustration. – Crystal structure illustrations of the ball-and-stick type are made up of three components: balls (atoms), sticks (bonds), and labels. The three components are drawn with the 700, 800, and 900 instruction series respectively; the first two instruction series can also perform certain types of labeling.

A new instruction 511 in the OR TEP-II version of the program was added to store information needed for the overlap correction. This instruction is used before the 700 and 800 series instructions.

The atom representation can be either a general ellipsoid or a boundary ellipse. In some cases these become a sphere and a circle. Chemical symbols may be plotted simultaneously with the atoms.

For our example we might simply draw circles and put the chemical symbols within the circles by using instruction 704 (see 3.3.8.1). This instruction will draw all the atoms of the subject and their chemical symbols.

The bonds are not always necessary in a drawing, but for structures with molecules or with distinctive groupings they are usually quite helpful. The most convenient method for describing and drawing bonds is instruction 812 (see 3.3.9.2). This instruction uses vector search codes (see 3.1.5) which reflect the user's knowledge of the structural chemistry and the interatomic distance ranges for the compound being drawn. Covalent bonds or any other desired type are found and drawn automatically from the list of atoms which make up the subject. If desired, the interatomic distance label can also be drawn with each bond (see 3.3.9).

Various types of labeling can be done with the 900 series instruction. The one which will most often be included is a caption for the figure, using instruction 902 (see 3.3.10.2).

2.2.5 Terminating the Drawing of the Illustration. – The plotter control instruction 202 (see 3.3.3.2) allows the user to remove the finished drawing from the plotting area and to place a fresh area of plot paper in position for any additional plots which may be drawn.

To terminate the computer job, a (--1) instruction (see 3.3.12) is used as the last instruction of the program.

2.3 Programming a Stereoscopic Illustration for OR TEP

A stereoscopic pair of figures is simply two perspective views of the subject as seen from two different viewpoints (which are usually about 6° apart). This pair is produced with OR TEP by programming for two drawings. A few additional instructions supplementary to those outlined in 2.2 are useful for producing stereo figures. These instructions are the stereoscopic rotation instruction 503 and the 1100 series of instructions, which facilitate the repetition of a series of instructions.

2.3.1 Stereoscopic Rotations. – In general, one member of a detailed stereoscopic illustration cannot be drawn completely independent of the other member of the pair because certain features (e.g., which octant of an ellipsoid is shaded) must be done identically in the two drawings. In OR TEP the "stereoscopically sensitive decisions" are handled by using two Cartesian coordinate systems: the reference Cartesian system and the working Cartesian system (see 3.1.8). The steps involved in picture composition (see 2.2.3) and the stereoscopically sensitive decisions are always based on the reference system, but the drawing of the illustration (see 2.2.4) is always based on the working system. A stereoscopic rotation is simply a rotation of the working system *from the reference system* about the axis which is vertical while viewing the final result. For example, a nominal rotation of +3° about the plotter y axis might be used for the left-eye view and a rotation of −3° about the same axis might be made before plotting the right-eye view, thus producing a total interocular angle of 6°.

A program to draw a stereo pair would involve the following steps:

1. preliminary graphical details,
2. composition of subject,
3. left-eye stereo rotation,
4. draw the subject,
5. advance the plotter,
6. right-eye stereo rotation,
7. draw the subject,
8. advance the plotter,
9. terminate the job.

2.3.2 Repeating a Sequence of Operations. – It should be noted that steps 7 and 8 in the stereo program of the last section are identical to steps 4 and 5. The program can be shortened somewhat by using the "saved sequence" instructions (see 3.3.11). A 1101 instruction (start saved sequence) would be placed between 3 and 4, and a 1102 instruction (end saved sequence) between 5 and 6. Then steps 7 and 8 can be replaced by a 1103 instruction (execute saved sequence).

Any sequence of instructions can be saved in this manner and repeated as many times as desired with 1103 instructions. For example, the saved sequence feature can be used to produce a complete series of views of a structure at (say) 15° intervals about an axis. Note that the instructions between the start and stop instructions are *both executed and saved* the first time through.

2.4 Drawing the Cubane Structure: An Example

The novel compound cubane[4] (C_4H_4) has been crystallized and the structure determined.[5] The carbon-carbon bonds lie along the edges of a cube within experimental error. The compound crystallizes with the trigonal symmetry of space group $R\bar{3}$. One carbon and one hydrogen are in special positions along the $\bar{3}$ axis, and the remaining carbon and hydrogen are in general positions. Anisotropic temperature factor coefficients were fitted to the carbon atoms during the least-squares refinement of the structure, and isotropic temperature factors were used for the hydrogen atoms.

The cell parameters are

$$a = b = c = 5.34\ \text{A}\ ,$$

$$\alpha = \beta = \gamma = 72.26^\circ\ .$$

The equivalent positions of space group[6] $R\bar{3}$ are x,y,z; z,x,y; y,z,x; $\bar{x},\bar{y},\bar{z}$; $\bar{z},\bar{x},\bar{y}$; and $\bar{y},\bar{z},\bar{x}$.

The positional parameters for C1, C2, H1, and H2 are given as −0.18711, 0.19519, 0.10706; 0.11546, 0.11546, 0.11546; −0.3246, 0.3468, 0.1848; and 0.2100, 0.2100, 0.2100, respectively. The anisotropic temperature factors given for the carbon atoms are of the type called zero[7] in this report (see 3.2.4.2). The coefficients b_{11}, b_{22}, b_{33}, b_{12}, b_{13}; b_{23} for C1 and C2 are 0.0410, 0.0425, 0.0450, −0.0042, −0.0142, −0.0051; and 0.0468, 0.0468, 0.0468, −0.0143, −0.0143, −0.0143.

2.4.1 Data Input for Cubane

2.4.1.1 Title Card (see 3.2.1). – FORMAT (12A6)

Card No.

(1) CUBANE (E. B. FLEISCHER (1964) J. A. C. S. 86, 3889)

2.4.1.2 Cell Parameter Card (see 3.2.2). – FORMAT (6F9.6)

(2)	5.34	5.34	5.34	72.26	72.26	72.26

2.4.1.3 Symmetry Cards (see 3.2.3)

FORMAT (I1, F14.10, 3F3.0, 2(F15.10, 3F3.0))

(3)	0	0.	1	0	0	0.	0	1	0	0.	0	0	1
(4)	0	0.	0	0	1	0.	1	0	0	0.	0	1	0

---

[4] P. Eaton and T. Cole, *J. Am. Chem. Soc.* **86**, 3157 (1964).

[5] E. B. Fleischer, *J. Am. Chem. Soc.* **86**, 3889 (1964).

[6] N. F. M. Henry and K. Lonsdale (eds.), *International Tables for X-Ray Crystallography*, vol. 1, Kynoch, Birmingham, 1962.

[7] Unfortunately, many authors of structure papers neglect to define the equation for the anisotropic temperature factor coefficients. In the present case, the type can be determined from the comparative isotropic temperature factor listed in anisotropic form in their Table I. In other instances one must arbitrarily choose a type (usually 0, 1, or 4 in the U.S.A.) and do the principal axis transformation, then check that the principal values are correct, or at least reasonable. In particular, the principal values must all be positive.

```
Card No.
  (5)      0        0.  0  1  0        0.  0  0  1        0.  1  0  0
  (6)      0        0. -1  0  0        0.  0 -1  0        0.  0  0 -1
  (7)      0        0.  0  0 -1        0. -1  0  0        0.  0 -1  0
  (8)      1        0.  0 -1  0        0.  0  0 -1        0. -1  0  0
```

2.4.1.4 Atomic Parameter Cards. –

Positional parameters (see 3.2.4.1): FORMAT (A6, 3X, 5F9.6, F9.0)

Thermal parameters (see 3.2.4.2): FORMAT (I1, F8.6, 5F9.6, F9.0)

Atoms 1 and 2 are entered with positional parameters type 0 and anisotropic temperature factors type 0.

```
Card No.
  (9)          C1                                        -.18711    .19519    .10706   0
 (10)     0          .04100    .04250    .04500    -.00420   -.01420   -.00510   0
 (11)          C2                                         .11546    .11546    .11546   0
 (12)     0          .04680    .04680    .04680    -.01430   -.01430   -.01430   0
```

Atoms 3 and 4 are entered with positional parameters type 0 and with dummy sphere temperature factors (type 7) 0.1 A in radius.

```
 (13)          H1                                        -.32460    .34680    .18480   0
 (14)     0          .1                                                                 7
 (15)          H2                                         .21000    .21000    .21000   0
 (16)     0          .1                                                                 7
```

Atom 5 is a dummy atom at the cell origin with a blank card dummy sphere (see next to last paragraph of 3.2.4.2). This could also be entered with type 7 as were atoms 3 and 4.

```
 (17)          ORGN                                       .00000    .00000    .00000   0
 (18)     1                                                                             0
```

In the card deck for this sample program, extensive use of Format No. 3 trailer cards (see 3.3.1.4) is made as a method of including a comment with an instruction. This convention is not mandatory, but it is a convenient method for annotating a program. This example uses a wide range of instructions in order to demonstrate them. As in the case with any programming system, there are many ways of doing any given problem. The Formats are described in Sect. 3.3.

2.4.2 Analysis of Structure (see 3.3.2). – These instructions are not connected with producing the figure. They are shown here just to demonstrate how they are used. A 101 instruction is used to obtain a tabulation of the atoms surrounding one atom or a series of several designated atoms. To obtain a list of all atoms (hydrogen and carbon atoms) out to a limit of (say) 3.61 A about the two carbons C1 and C2, one would use the following instruction. (The notation is explained in Sect. 3.3.2.)

Card No.

(19) 101 $\underbrace{155501\quad 2}_{}$ $\underbrace{1\qquad\qquad 4}_{}$ $\underbrace{3.61}_{}$

	Atoms 1 through 2 of symmetry operation 1	Atoms 1 through 4 of all symmetry and translation operations	*D* max

A 102 instruction gives both interatomic distances and interatomic angles. In order to find all covalent bonds and bond angles about the two carbons we might use the following instruction.

(20) 102 155501 2 1 4 1.8

In this case a smaller *D* max was used so that only the distances and angles of immediate interest would be computed.

2.4.3 Programming the Cubane Illustration. – First we must initialize the plotter package.

(21) 201

The two plot boundary dimensions can be equal for the present illustration since the cubane molecule is a cube. Suppose we use an 11- by 11-in. boundary and specify a 1.5-in. margin to give a total working area of 9 by 9 in. A 30-in. view distance might be reasonable to use in viewing a model of this size.

(22) 301 11 11 30 1.5

In general we would use retracing to make the lettering, and certain other details, stand out more prominently. However, for the test example we will eliminate the retracing so that the illustration will plot as fast as possible.

(23) 303 0

The subject of the illustration is a single cubane molecule, which we will now define. One way of designating this subject is to specify a sphere of enclosure, centered on the dummy atom 555501, which is at the center of a cubane molecule. A radius of 3.2 A should be adequate to isolate a single molecule.

Card No.

(24) $402\ \underbrace{555501\quad 5}_{(a)}\qquad \underbrace{1\qquad\qquad 4}_{(b)}\qquad \underbrace{3.2\quad}_{(c)}$

where the several parts designate:

(a) a run of origin atom (center of sphere) from atom 5 to atom 5 in symmetry position 55501 (that is, in this example, a single sphere),

(b) a run of target atom from atom 1 to atom 4, and

(c) a sphere radius of 3.2 A.

To orient the molecule, we will first define a coordinate system along the edges of the cubane cube. We will then rotate the molecule relative to this coordinate system to minimize overlap.

The origin of the coordinate system will be positioned on the dummy atom No. 5. The desired coordinate system orientation will be defined by specifying two vectors from the special position atom 255501 to the two symmetry-related general-position atoms 155501 and 155502.

(25) 501 555501 255501 155501 255501 155502 0 0

A rotation of 25° about the *Y* axis (axis 2) followed by a rotation of 28° about the *X* axis (axis 1) will produce a satisfactory view of the molecule.

(26) 502 2 25 1 28

To scale and position the subject for projection onto the drawing board and to utilize all available space, we will use the 604 instruction, which will automatically set X0, Y0, and SCAL1. However, the ellipsoid scale factor ratio SCAL2 must be specified independently. If we want thermal ellipsoids corresponding to 50% probability, then we will enter 1.54 for SCAL2.

(27) 604 0 0 0 1.54

This completes the composition of the illustration.

The stereoscopic rotation for the left eye can be done at this point. We will use a rotation of 2.7° about the *Y* axis (axis 2) for the left-eye view. Later in the program, we will make a –2.7° rotation about the same axis for the right-eye view to give a total interocular angle of 5.4°.

(28) 503 2 2.7

Since the structure will be drawn twice, once for each eye, the "saved sequence" feature can be used to shorten the program. Note that the instructions between the start

Card No.

and stop instructions are both *executed and saved* the first time through. They can then be re-executed as many times as desired by using the "execute saved sequence" instruction 1103.

The 1101 instruction starts the saved sequence.

(29) 1101

The 511 instruction stores the information needed for the overlap hidden-line correction (i.e., as projected boundary ellipses for each atom in the ATOMS list and a quadrangle approximation for each bond). The bonds are specified with a format No. 2 trailer card identical to that used in the 812 instruction described below.

(30) 2 511 0

(31) 0 1 4 1 4 4 0.9 1.6 .04

The ATOMS list currently contains all the atom designators for one cubane molecule. We want to draw the molecule in two separate steps so that the hydrogen and carbon atoms can be given different graphical representations. To draw the carbon atoms (ANR = 1, 2), we will construct a special code that (a) draws the three principal-plane forward traces and the boundary-plane trace (NPLANE = 4), (b) omits the reverse sides of the principal planes (NDOT = 0), (c) draws the forward principal axes without additional shading (NLINE = 1), and (d) omits the reverse principal axes (NDASH = 0). In addition we want the chemical symbols to be drawn with letters 0.2-in. high (before projection) and displaced from the atomic center by 0.6 in. in the horizontal direction and 0.7 in. in the vertical direction.

(32) 1 715 4 0 1 0 .2 .6 .7

(33) 0 0 0 1 2

The 715 instruction is used, rather than 705, to shorten the output listing of the example. Normally we would use the 705 to obtain a listing of all coordinates.

Since the hydrogen atoms (ANR = 3, 4) are to be drawn with a standard model, the construction details will be taken care of automatically. We want chemical symbols 0.2 in. high and offset 0.35 in. horizontally and 0.4 in. vertically.

(34) 1 712 0 0 0 0 .2 .35 .4

(35) 0 0 0 3 4

The most convenient procedure for drawing bonds is to use the implicit bond instruction 812. All other information can be entered with a single format No. 2 trailer card (vector search code card).

Card No.

(36) 2 812

(37) 0

$$\underbrace{1 \qquad 4}_{(a)} \quad \underbrace{1 \qquad 4}_{(b)} \quad \underbrace{4}_{(c)} \quad \underbrace{.9 \qquad 1.6}_{(d)} \quad \underbrace{.04}_{(e)}$$

where

(*a*) and (*b*) are atom number runs for atom-pair bonds to be drawn,

(*c*) denotes bond type 4,

(*d*) denotes the distance range 0.9 to 1.6 A, which will cover all covalent bond distances, and

(*e*) the bond radius, is 0.04 A.

The remaining fields in the card can be blank, since a complete set of bond distance labels is not desired.

Because of the symmetry, there are only two different C – C bond lengths in cubane. These are C1-C1 and C1-C2. We shall label one example of each of these bonds. For variety let us label one with a normal bond-length label and the other with a perspective label. The two bonds which can be labeled most advantageously are (*a*) 155504 → 155503 and (*b*) 255504 → 155505. The labels will be 0.15 in. in height and displaced vertically from the bond center by – 0.4 in.

(38) 906 155504 155503 0 0 .15 0 –.4

(39) 916 255504 155505 0 0 .15 0 –.4

The final feature to be drawn is a caption (CUBANE) for the illustration. This can conveniently be positioned by "hanging" it from the dummy atom 555501 and "bouncing" it 1 in. off the lower *y* boundary.

(40) 3 902 555501 0 0 1. .25 0 0

(41) CUBANE

The saved sequence can now be terminated.

(42) 1102

The plotter is then advanced 9 in. along *x* in preparation for the right-eye view.

(43) 202 9

The stereo rotation of –2.7° about axis 2 is now performed in preparation for the right-eye view. (Note that this rotation starts with the reference orientation, not the previous working orientation.)

(44) 503 2 –2.7

Card No.

The saved sequence can now be repeated for the right eye. Note that the atom list now contains the same information that it did when the first view was drawn.

(45) 1103

The illustration is now complete. The plotter is next advanced 20 in. along x to remove this figure from the working area.

(46) 202 20

A dummy plot for the CalComp system is now added to aid in stopping the CalComp plotter.

(47) 202 0

Finally we terminate the job and exit from the program.

(48) −1

2.4.4 **Stereoscopic Illustration of the Examples.** – Figure 2.1 shows the stereoscopic pair exactly as it was plotted by a mechanical CalComp system, except for photographic reduction. Figure 2.2 shows one-half of the same illustration at a larger scale. These drawings have not been retouched.

Note that one bond distance label was drawn in perspective along the bond, and the other was drawn as a regular label parallel to the page.

Figure 2.3 is an example of a figure without photographic reduction drawn by a CalComp plotter which has 0.005 in. step-size resolution. Another representation of the same structure is shown in Fig. 6.19.

The input data and OR TEP instructions for Fig. 2.3 are listed in 2.4.5.2. The user should examine this example carefully since several useful techniques are illustrated.

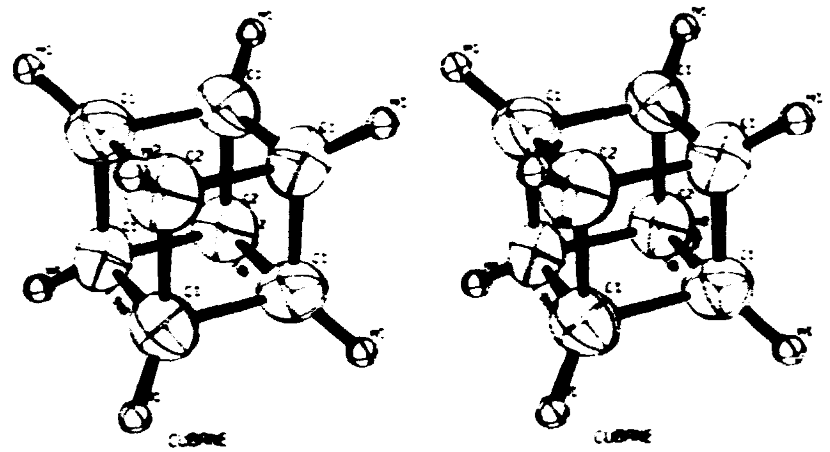

Fig. 2.1. The Sample Figure Cubane Reduced for Stereoscopic Viewing.

ORNL DWG 75 16856

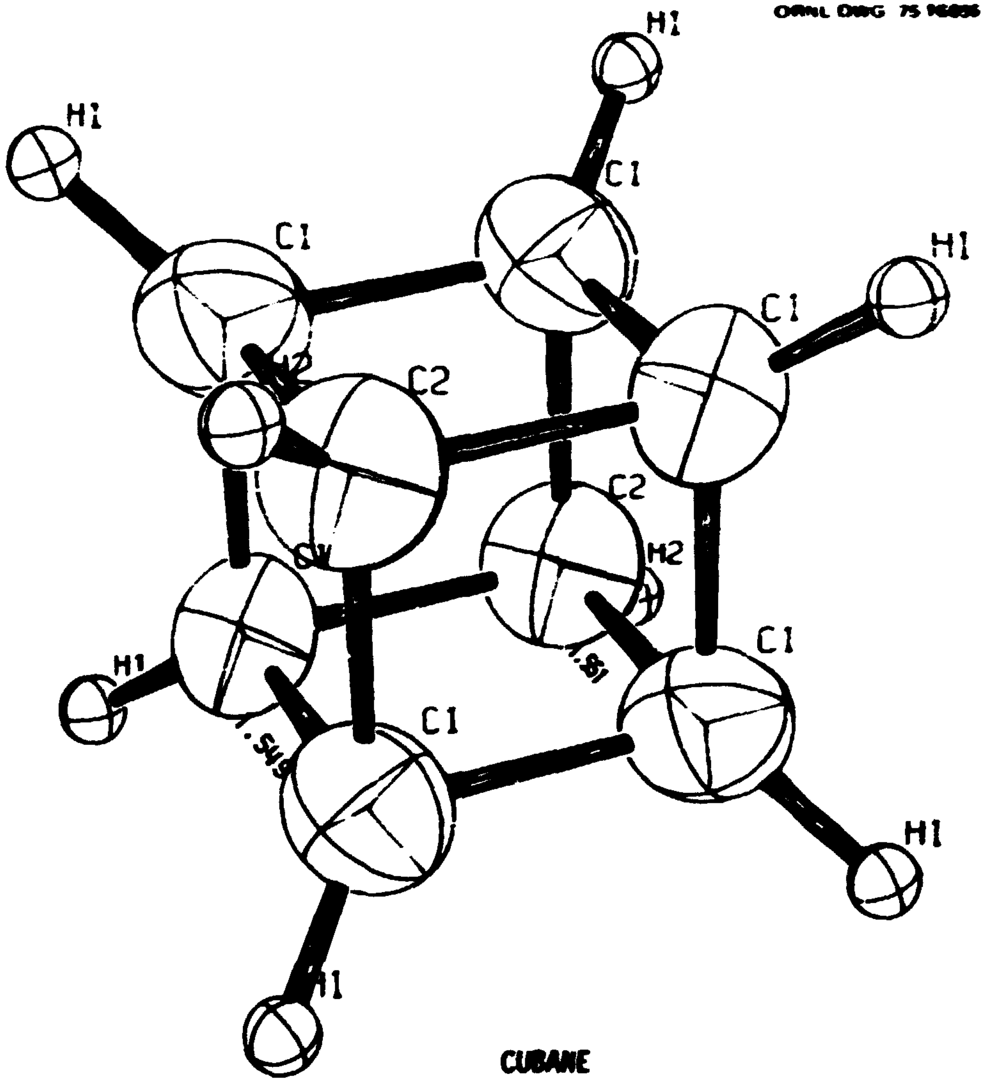

Fig. 2.2. The Sample Figure Cubane at 82% of Original Scale.

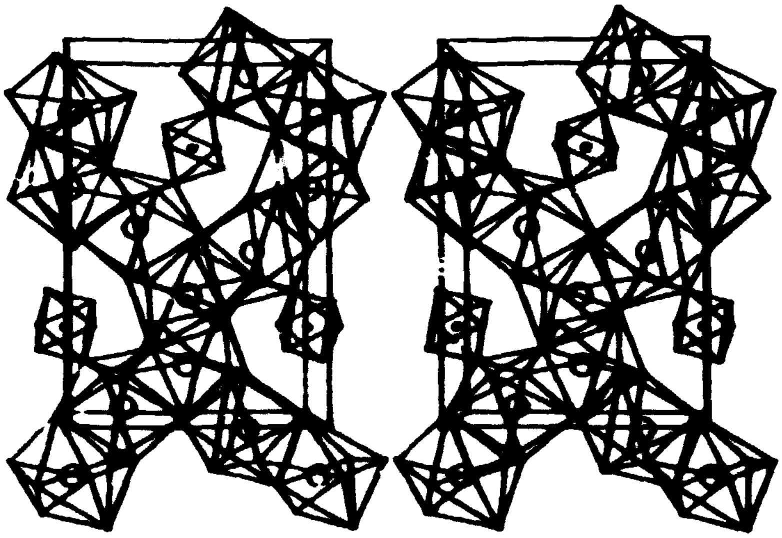

Fig. 2.3 Polyhedra Representation of Potassium Perxenate 9-Hydrate.

2.4.5 Listing of Sample Input and Output. – *2.4.5.1 Listing of Input Cards for Cubane.* –

```
CUBANE  E.B.FLEISCHER    1964  J.A.C.S.  86,3889                        EXAM  10
    5.34      5.34      5.34     72.26     72.26     72.26              EXAM  20
           0  1  0  0               0  0  1  0              0  0  0  1EXAM  30
           0  0  0  1               0  1  0  0              0  0  1  0EXAM  40
           0  0  1  0               0  0  0  1              0  1  0  0EXAM  50
           0 -1  0  0               0  0 -1  0              0  0  0 -1EXAM  60
           0  0  0 -1               0 -1  0  0              0  0 -1  0EXAM  70
1          0  0 -1  0               0  0  0 -1              0 -1  0  0EXAM  80
 C1                              -.10711    .19515    .10706   0        EXAM  90
  .04100    .04250    .04500    -.00420   -.01420   -.00510   0         EXAM 100
 C2                               .11546    .11546    .11546   0        EXAM 110
  .04633    .04600    .04600    -.01430   -.01430   -.01430   0         EXAM 120
 B1                              -.32460    .30600    .10400   0        EXAM 130
    .10                                                        7        EXAM 140
 B2                               .21000    .21000    .21000   0        EXAM 150
    .10                                                        7        EXAM 160
 ORGN                                  0         0         0   0        EXAM 170
1                                                              0        EXAM 180
  3   101   1555C1       2         1         4      3.61                EXAM 190
***** FIND ALL NEIGHBOR ATOMS AROUND C1 AND C2 OUT TO 3.61 A *****      EXAM 200
  3   102   1555C1       2         1         4      1.8                 EXAM 210
***** FIND COVALENT BONDS AND BOND ANGLES AROUND CARBONS *****          EXAM 220
  3   201                                                               EXAM 230
***** INITIALIZE MECHANICAL PLOTTER PACKAGE. 203 FOR CRT PACKAGE *****  EXAM 240
  3   301        11.       11.       30.      1.5                       EXAM 250
***** 11X11 BOUNDARY, ORG INSIDE 1.5 MARGIN, VIEW FROM 30 INCHES *****  EXAM 260
  3   303                                                               EXAM 270
***** ELIMINATE ALL RETRACING *****                                     EXAM 280
  3   402   555501       5         1         4      3.2                 EXAM 290
***** ENCLOSED SPHERE OF RADIUS 3.2 A ABOUT DUMMY ATOM 5,555,01 *****   EXAM 300
  3   501   555501   255501   155501   255501   155502                 0EXAM 310
***** ORIGIN ON DUMMY ATOM 555501, VECTORS ALONG 2 EDGES OF CUBANE *****EXAM 320
  3   502            2       25.         1      20.                     EXAM 330
***** ROTATE 25 DEGREES ABOUT Y, THEN 20 DEGREES ABOUT NEW X *****      EXAM 340
  3   604            0         0         0     1.50                     EXAM 350
***** AUTOMATIC SCALE AND POSITION, 50 PERCENT PROBABILITY ELLIPSOIDS **EXAM 360
  3   503            2       2.7                                        EXAM 370
```

```
***** STEREO ROTATION OF 2.7 DEGREES ABOUT Y FOR LEFT EYE *****          EXAM 380
  3  1101                                                                EXAM 390
***** START SAVE SEQUENCE *****                                          EXAM 400
  2   511          0                                                     EXAM 410
  3         1  4  1  4  4   0.9   1.6   .04                              EXAM 420
***** STORE PROJECTED ATOMS AND BONDS FOR OVERLAP, MARGIN SET BY DEFAULTEXAM 430
  1   715          4          0          1          0       .20      .60       .73EXAM 440
  3                                      1          2                    EXAM 450
***** DRAW CARBON ATOM ELLIPSOIDS, ATOM NUMBER RUN 1-2 *****             EXAM 460
  1   712                                               .20      .35       .40EXAM 470
  3                                      3          4                    EXAM 480
***** DRAW HYDROGEN ATOM SPHERES, ATOM NUMBER RUN 3-4 *****              EXAM 490
  2   812                                                                EXAM 500
  3         1  4  1  4  4   0.9   1.6   .04                              EXAM 510
***** TYPE 4 BONDS .04 A BOND RADIUS, ATOMS 1-4 TO ATOMS 1-4, 0.9-1.6 A EXAM 520
  3   906    155504    155503          0          0       .15          0      -.0EXAM 530
***** LABEL BOND 155504-155503 WITH REGULAR BOND DISTANCE LABEL *****    EXAM 540
  3   916    255504    155505          0          0       .15          0      -.0EXAM 550
***** LABEL BOND 255504-155505 WITH PERSPECTIVE BOND DISTANCE LABEL ****EXAM 560
  3   902    555501          0          0        1.0       .25          0       3EXAM 570
                                      CUBANE                             EXAM 580
  3  1102                                                                EXAM 590
***** END OF SAVE SEQUENCE *****                                         EXAM 600
  3   202          5.                                                    EXAM 610
***** ADVANCE PLOTTER 9 INCHES ALONG X *****                             EXAM 620
  3   503          2      -2.7                                           EXAM 630
***** STEREO ROTATION OF -2.7 DEGREES ABOUT Y FOR RIGHT EYE VIEW *****   EXAM 640
  3  1103                                                                EXAM 650
***** EXECUTE SAVED SEQUENCE FOR RIGHT EYE DRAWING *****                 EXAM 660
  3   232        20.                                                     EXAM 670
***** ADVANCE PLOTTER 20 INCHES *****                                    EXAM 680
  3   202                                                                EXAM 690
***** ADD DUMMY BLOCK TO MAGNETIC TAPE *****                             EXAM 700
     -1                                                                  EXAM 710
```

2.4.5.2 Listing of Input Cards for Potassium Perxenate 9-Hydrate. —

```
POTASSIUM PERXENATE 9-HYDRATE/A.ZALKIN ET AL /(1964) JACS 86,3569         EXAM0010
   9.363    13.224    15.616       90.       90.       90.                 EXAM0020
            .0  1  0  0               .0  0  1  0               .0  0  0  1EXAM0030
            .0 -1  0  0               .0  0 -1  0               .5  0  0  1EXAM0040
            .0 -1  0  0               .5  0  1  0               .0  0  0  1EXAM0050
1           .0  1  0  0               .5  0 -1  0               .5  0  0  1EXAM0060
 XE                          .262      .000      .250                      EXAM0070
      .13                                                     7            EXAM0080
 K1                          .024      .987      .539                      EXAM0090
      .37                                                     7            EXAM0100
 K2                          .046      .234      .554                      EXAM0110
      .37                                                     7            EXAM0120
 K3                          .397      .227      .024                      EXAM0130
      .33                                                     7            EXAM0140
 K4                          .077      .989      .139                      EXAM0150
      .37                                                     7            EXAM0160
 C1                          .633      .101      .251                      EXAM0170
      .27                                                     7            EXAM0180
 C2                          .096      .074      .253                      EXAM0190
      .27                                                     7            EXAM0200
 C3                          .139      .096      .316                      EXAM0210
      .27                                                     7            EXAM0220
 C4                          .176      .058      .151                      EXAM0230
      .27                                                     7            EXAM0240
 C5                          .329      .319      .351                      EXAM0250
      .27                                                     7            EXAM0260
```

```
 Co                                .360     .881      .189                      EXAP0270
     .23                                                          7             EXAP0280
 W1                                .654     .839      .193                      EXAP0290
     .23                                                          7             EXAP0300
 W2                                .850     .136      .297                      EXAP0310
     .23                                                          7             EXAP0320
 W3                                .873     .029      .369                      EXAP0330
     .23                                                          7             EXAP0340
 W4                                .692     .046      .536                      EXAP0350
     .23                                                          7             EXAP0360
 W5                                .997     .243      .111                      EXAP0370
     .23                                                          7             EXAP0380
 W6                                .967     .980      .572                      EXAP0390
     .23                                                          7             EXAP0400
 W7                                .376     .470      .002                      EXAP0410
     .23                                                          7             EXAP0420
 W8                                .493     .262      .806                      EXAP0430
     .23                                                          7             EXAP0440
 W9                                .606     .150      .124                      EXAP0450
     .23                                                          7             EXAP0460
ORGN                               .250     .500      .400                      EXAP0470
     .13                                                          7             EXAP0480
                                   .000     .000      .000                      EXAP0490
1    .03                                                          7             EXAP0500
  3  102   155501   555501        1        20     3.55                          EXAP0510
***** DISTANCES,ANGLES AND EDGES OF KE AND S COORDINATION POLYHEDRA ****EXAP0520
  3  201                                                                        EXAP0530
***** INITIALIZE CALCOMP PLOT PACKAGE *****                                     EXAP0540
  3  301        10        11        12     7.05                                 EXAP0550
***** 10-20-.95 = 2.3 IN. DIAMETER PICTURES,12 IN. AWAY,DIRECT STEREO VUEXAP0560
  3  401  2255501 -2260601                                                      EXAP0570
***** STORE UNIT CELL CORNERS FOR CELL OUTLINE *****                            EXAP0580
  3  406        21        21        1         5      .13      .52      .57EXAP0590
***** STORE CENTRAL ATOMS OF POLYHEDRA ****                                     EXAP0600
  3  405         1         5        1        20     3.52                        EXAP0610
***** CONSTRUCT SPHERE OF ENCLOSURE WITH EACH CENTRAL ATOM *****                EXAP0620
  3  501  1155501  2155501  2156501  2155501  2156601                          1EXAP0630
***** B AXIS HORIZONTAL, C AXIS VERTICAL, VIEWED ALONG -A AXIS *****            EXAP0640
  3  506                                                                        EXAP0650
***** AUTOMATIC SCALE AND POSITION *****                                        EXAP0660
  3  503         2         3                                                    EXAP0670
***** STEREO ROTATION FOR LEFT EYE VIEW *****                                   EXAP0680
  3 1101                                                                        EXAP0690
***** START SAVED SEQUENCE *****                                                EXAP0700
  1  716                                                                        EXAP0710
  3                                 1         5                                 EXAP0720
***** DRAW METAL ATOMS SELECTIVELY *****                                        EXAP0730
  2  815                                                                        EXAP0740
  2       22 22 22 22  1   9.0  11.0   .01                                      EXAP0750
  2       22 22 22 22  1  15.5  16.0   .01                                      EXAP0760
  2        5 11  5 11  1   2.5   2.9   .04    -1     1    1.8    1.9            EXAP0770
  2        5 19  5 19  1   2.6   4.4   .02    -2     2    2.6    3.1            EXAP0780
  2       17 23 17 23  1   2.6   4.7   .02    -3     3    2.7    3.52           EXAP0790
  2        9 23  9 23  1   2.6  4.50   .02    -4     4    2.7    3.3            EXAP0800
  2        7 23  7 23  1   2.6   4.6   .02    -5     5    2.7    3.2            EXAP0810
***** DRAW POLYHEDRA AND CELL OUTLINE *****                                     EXAP0820
  3 1102                                                                        EXAP0830
***** END SAVED SEQUENCE *****                                                  EXAP0840
  3  202       2.4                                                              EXAP0850
***** ADVANCE PLOTTER FOR RIGHT EYE VIEW *****                                  EXAP0860
  3  503         2        -3                                                    EXAP0870
***** STEREO ROTATION FOR RIGHT EYE VIEW *****                                  EXAP0880
  3 1105                                                                        EXAP0890
***** REPEAT SAVED SEQUENCE                                                     EXAP0900
  3  202        10                                                              EXAP0910
***** ADVANCE PLOTTER 10 IN. *****                                              EXAP0920
  3  202                                                                        EXAP0930
***** ADD DUMMY PLOT ( STOP CALCOMP ON PLOT NO. 3 ) *****                       EXAP0940
      -1                                                                        EXAP0950
```

2.4.5.3 *Listing of Output from the Monitor Output Tape of the Computer.* –

```
  CUBANE  E.B.FLEISCHER   1964  J.A.C.S.  86,3889

 DIRECT CELL PARAMETERS
     A               B              C             ALPHA          BETA          GAMMA
 5.339999        5.339999       5.339999         72.260         72.260         72.260
                                       COSINE 0.30469871     0.30469871     0.30469071

 RECIPROCAL CELL PARAMETERS
     A*              B*             C*            ALPHA*         BETA*          GAMMA*
 0.202207        0.202207       0.202207        103.506        103.506        103.506
                                       COSINE -0.23353952    -0.23353940    -0.23353940

 SYMMETRY TRANSFORMATIONS
      NO.              TRANSFORMED X                    TRANSFORMED Y                    TRANSFORMED Z
       1      0.0       1. X  0. Y  0. Z      0.0       0. X  1. Y  0. Z       0.0       0. X  0. Y  1. Z
       2      0.0       0. X  0. Y  1. Z      0.0       1. X  0. Y  0. Z       0.0       0. X  1. Y  0. Z
       3      0.0       0. X  1. Y  0. Z      0.0       0. X  0. Y  1. Z       0.0       1. X  0. Y  0. Z
       4      0.0      -1. X  0. Y  0. Z      0.0       0. X -1. Y  0. Z       0.0       0. X  0. Y -1. Z
       5      0.0       0. X  0. Y -1. Z      0.0      -1. X  0. Y  0. Z       0.0       0. X -1. Y  0. Z
       6      0.0       0. X -1. Y  0. Z      0.0       0. X  0. Y -1. Z       0.0      -1. X  0. Y  0. Z

NO. ATOM       X           Y           Z               B11        B22        B33        B12        B13        B23     TYPE
 1   C1    -0.187110   0.195190    0.107060        0.041060   0.042500   0.045000  -0.004200  -0.014200  -0.005100   8.
 2   C2     0.115460   0.115460    0.115460        0.046800   0.046800   0.046800  -0.014300  -0.014300  -0.014300   0.
 3   H1    -0.324600   0.346800    0.184800        0.100000   0.0        0.0        0.0        0.0        0.0        7.
 4   H2     0.210000   0.210000    0.210000        0.100000   0.0        0.0        0.0        0.0        0.0        7.
 5  ORGN    0.0        0.0         0.0             0.0        0.0        0.0        0.0        0.0        0.0        0.

NO. ATOM       X           Y           Z              RMSD 1     RMSD 2     RMSD 3
 1   C1    -0.187110   0.195190    0.107060        0.204099   0.239056   0.255794
 2   C2     0.115460   0.115460    0.115460        0.205704   0.247732   0.247732
 3   H1    -0.324600   0.346800    0.184800        0.100000   0.100000   0.100000
 4   H2     0.210000   0.210000    0.210000        0.100000   0.100000   0.100000
 5  ORGN    0.0        0.0         0.0             0.100000   0.100000   0.100000
```

```
     CUBANE E.B.FLEISCHER   1964  J.A.C.S.  86,3889

     ORTHONORMAL REFERENCE VECTORS BASED ON CRYSTAL AXES               POST-FACTOR TRANSFORMATION MATRIX
          X VECTOR         Y VECTOR         Z VECTOR
       0.1072659E 00  -0.5990040E-01  -0.4722326E-01          0.5339996E 01   0.9536743E-06   0.9536743E-06
       0.0              0.1966153E 00  -0.4722320E-01          0.1627090E 01   0.5086076E 01   0.9536743E-06
       0.0              0.0              0.2022060E 00          0.1627090E 01   0.1107799E 01   0.4945430E 01

((((( INSTRUCTION  101 )))))
      0.1555010E 06  0.2000000E 01  0.1000000E 01  0.4000000E 01  0.3610000E 01  0.0           0.0

     ***** FIND ALL NEIGHBOR ATOMS AROUND C1 AND C2 OUT TO 3.61 A *****

          FROM ATOMS    TO ATOMS     WITH RADIUS OR, IF A BOX, WITH SEMIDIMENSIONS
     CODE   (MIN  MAX)   (MIN  MAX)                          A         B         C

     101  155501   255501   1   4                        3.610     0.0       0.0

     VECTORS FROM ATOM  (  1,55501)       TO ATOMS   1 THROUGH   4
          C1     H1     (  1,55501)-0.1071 0.1952 0.1071       (  3,55501)-0.3246 0.3468 0.1048         D = 1.012
          C1     C1                                            (  1,55505)-0.1071 0.1071-0.1952         D = 1.549
          C1     C1                                            (  1,55506)-0.1952-0.1071 0.1071         D = 1.549
          C1     C2                                            (  2,55501) 0.1155 0.1155 0.1155         D = 1.552
          C1     C1                                            (  1,55502) 0.1071-0.1071 0.1952         D = 2.103
          C1     C1                                            (  1,55503) 0.1952 0.1071-0.1071         D = 2.103
          C1     C2                                            (  2,55504)-0.1155-0.1155-0.1155         D = 2.202
          C1     H1                                            (  3,55506)-0.3468-0.1048 0.3246         D = 2.202
          C1     H1                                            (  3,55505)-0.1048 0.3246-0.3468         D = 2.306
          C1     H2                                            (  4,55501) 0.2100 0.2100 0.2100         D = 2.376
          C1     C1                                            (  1,55504) 0.1071-0.1952-0.1071         D = 2.677
          C1     H1                                            (  3,55502) 0.1048-0.3246 0.3468         D = 3.052
          C1     H1                                            (  3,55503) 0.3468 0.1048-0.3246         D = 3.069
          C1     H2                                            (  4,45501)-0.7900 0.2100 0.2100         D = 3.077
          C1     H2                                            (  4,56504)-0.2100 0.7900-0.2100         D = 3.096
          C1     H2                                            (  4,55504)-0.2100-0.2100-0.2100         D = 3.175
          C1     H1                                            (  3,55605)-0.1048 0.3246 0.6532         D = 3.200
          C1     H1                                            (  3,45603)-0.6532 0.1048 0.6754         D = 3.204
          C1     H1                                            (  3,46504)-0.6754 0.6532-0.1048         D = 3.300
          C1     C2                                            (  2,56504)-0.1155 0.8845-0.1155         D = 3.609

     VECTORS FROM ATOM  (  2,55501)       TO ATOMS   1 THROUGH   4
          C2     H2     (  2,55501) 0.1155 0.1155 0.1155       (  4,55501) 0.2100 0.2100 0.2100         D = 1.109
          C2     C1                                            (  1,55501)-0.1071 0.1952 0.1071         D = 1.552
          C2     C1                                            (  1,55502) 0.1071-0.1071 0.1952         D = 1.552
          C2     C1                                            (  1,55503) 0.1952 0.1071-0.1071         D = 1.552
          C2     C1                                            (  1,55504) 0.1071-0.1952-0.1071         D = 2.202
          C2     C1                                            (  1,55505)-0.1071 0.1071-0.1952         D = 2.202
          C2     C1                                            (  1,55506)-0.1952-0.1071 0.1071         D = 2.202
          C2     H1                                            (  3,55501)-0.3246 0.3468 0.1048         D = 2.273
          C2     H1                                            (  3,55502) 0.1048-0.3246 0.3468         D = 2.273
          C2     H1                                            (  3,55503) 0.3468 0.1048-0.3246         D = 2.273
          C2     C2                                            (  2,55504)-0.1155-0.1155-0.1155         D = 2.710
          C2     H1                                            (  3,55504) 0.3246-0.3468-0.1048         D = 3.091
          C2     H1                                            (  3,55505)-0.1048 0.3246-0.3468         D = 3.091
          C2     H1                                            (  3,55506)-0.3468-0.1048 0.3246         D = 3.091
          C2     H1                                            (  3,56504) 0.3246 0.6532-0.1048         D = 3.101
          C2     H1                                            (  3,55605)-0.1048 0.3246 0.6532         D = 3.101
          C2     H1                                            (  3,65506) 0.6532-0.1048 0.3246         D = 3.101
          C2     C1                                            (  1,56504) 0.1071 0.8048-0.1071         D = 3.609
          C2     C1                                            (  1,55605)-0.1071 0.1071 0.8048         D = 3.609
          C2     C1                                            (  1,65506) 0.8048-0.1071 0.1071         D = 3.609
```

```
((((( INSTRUCTION  102 )))))
      0.1555010E 06  0.2000000E 01  0.1000000E 01  0.4000000E 01  0.1799999E 01  0.0            0.0

     ***** FIND COVALENT BONDS AND BOND ANGLES AROUND CARBONS *****

            FROM ATOMS     TO ATOMS      WITH RADIUS OR, IF A BOX, WITH SEMIDIMENSIONS
     CODE   (MIN  MAX)   (MIN  MAX)                                A        B         C

     102  155501   255501   1   4                           1.800    0.0      0.0


     VECTORS FROM ATOM  (  1,55501)        TO ATOMS   1 THROUGH   4
          C1     H1     (  1,55501)-0.1871 0.1952 0.1071        (  3,55501)-0.3246 0.3468 0.1848        D = 1.012
          C1     C1                                             (  1,55505)-0.1071 0.1871-0.1952        D = 1.549
          C1     C1                                             (  1,55506)-0.1952-0.1071 0.1871        D = 1.549
          C1     C2                                             (  2,55501) 0.1155 0.1155 0.1155        D = 1.552

     ANGLES AROUND ATOM    1
          H1     C1     C1          (  3,55501) (  1,55501) (  1,55505)              D = 2.282       A =124.69
          H1     C1     C1          (  3,55501) (  1,55501) (  1,55506)              D = 2.306       A =127.16
          H1     C1     C2          (  3,55501) (  1,55501) (  2,55501)              D = 2.273       A =123.52
          C1     C1     C1          (  1,55505) (  1,55501) (  1,55506)              D = 2.183       A = 89.60
          C1     C1     C2          (  1,55505) (  1,55501) (  2,55501)              D = 2.202       A = 90.48
          C1     C1     C2          (  1,55506) (  1,55501) (  2,55501)              D = 2.202       A = 90.48

     VECTORS FROM ATOM  (  2,55501)        TO ATOMS   1 THROUGH   4
          C2     H2     (  2,55501) 0.1155 0.1155 0.1155        (  4,55501) 0.2100 0.2100 0.2100        D = 1.109
          C2     C1                                             (  1,55501)-0.1071 0.1952 0.1071        D = 1.552
          C2     C1                                             (  1,55502) 0.1071-0.1871 0.1952        D = 1.552
          C2     C1                                             (  1,55503) 0.1952 0.1071-0.1871        D = 1.552

     ANGLES AROUND ATOM    2
          H2     C2     C1          (  4,55501) (  2,55501) (  1,55501)              D = 2.376       A =125.66
          H2     C2     C1          (  4,55501) (  2,55501) (  1,55502)              D = 2.376       A =125.66
          H2     C2     C1          (  4,55501) (  2,55501) (  1,55503)              D = 2.376       A =125.66
          C1     C2     C1          (  1,55501) (  2,55501) (  1,55502)              D = 2.183       A = 89.44
          C1     C2     C1          (  1,55501) (  2,55501) (  1,55503)              D = 2.183       A = 89.44
          C1     C2     C1          (  1,55502) (  2,55501) (  1,55503)              D = 2.183       A = 89.44
((((( INSTRUCTION  201 )))))
      0.0            0.0            0.0            0.0            0.0            0.0            0.0

     ***** INITIALIZE MECHANICAL PLOTTER PACKAGE. 203 FOR CRT PACKAGE *****

((((( INSTRUCTION  301 )))))
      0.1100000E 02  0.1100000E 02  0.3600000E 02  0.1500000E 01  0.0            0.0            0.0

     ***** 11X11 BOUNDARY, 8X8 INSIDE 1.5 MARGIN, VIEW FROM 30 INCHES *****

     PLOT LIMITS 11.00 BY 11.00 IN.  INCLUDING  1.50  IN. MARGIN
     VIEW DISTANCE 30.000 INCHES
```

```
((((( INSTRUCTION  303 )))))
    0.0           0.0           0.0           0.0           0.0           0.0           0.0

     ***** ELIMINATE ALL RETRACING *****

     RETRACE DISPLACEMENT = 0.0    INCH

((((( INSTRUCTION  402 )))))
    0.5555010E 06  0.5000000E 01  0.1000000E 01  0.4000000E 01  0.3200000E 01  0.0           0.0

     ***** ENCLOSE SPHERE OF RADIUS 3.2 A ABOUT DUMMY ATOM 5,555,01 *****

            FROM ATOMS     TO ATOMS     WITH RADIUS OR, IF A BOX, WITH SEMIDIMENSIONS
     CODE   (MIN  MAX)    (MIN  MAX)                        A         B         C
     402  555501   555501    1   4                       3.200      0.0       0.0

     VECTORS FROM ATOM  (  5,55501)       TO ATOMS   1 THROUGH   4

     CONTENTS OF ATOMS ARRAY
            155501.   255501.   355501.   455501.   155502.   355502.   155503.   355503.   155504.   255504.
            355504.   455504.   155505.   355505.   155506.   355506.

((((( INSTRUCTION  501 )))))
    0.5555010E 06  0.2555010E 06  0.1555010E 06  0.2555010E 06  0.1555020E 06  0.0           0.0

     ***** ORIGIN ON DUMMY ATOM 555501, VECTORS ALONG 2 EDGES OF CUBANE *****

     ORIGIN FOR PROJECTION AXIS IN CRYSTAL COORD.       0.0           0.0           0.0

     ORTHONORMAL REFERENCE VECTORS BASED ON CRYSTAL AXES               POST-FACTOR TRANSFORMATION MATRIX
          X VECTOR          Y VECTOR         Z VECTOR
       -0.1950173E 00  -0.5332431E-01   0.3517690E-02          -0.5161572E 01   0.2120973E 00   0.1352190E 01
        0.5133009E-01   0.4031152E-02   0.1955263E 00          -0.2760960E 00   0.1350079E 01   0.5159129E 01
       -0.5414121E-02   0.1954785E 00  -0.5144400E-01          -0.1402325E 01   0.5145890E 01   0.2624693E 00

((((( INSTRUCTION  502 )))))
    0.2000000E 01  0.2500000E 02  0.1000000E 01  0.2800000E 02  0.0           0.0           0.0

     ***** ROTATE 25 DEGREES ABOUT Y, THEN 28 DEGREES ABOUT NEW X *****

     ORIGIN FOR PROJECTION AXIS IN CRYSTAL COORD.       0.0           0.0           0.0

     ORTHONORMAL REFERENCE VECTORS BASED ON CRYSTAL AXES               POST-FACTOR TRANSFORMATION MATRIX
          X VECTOR          Y VECTOR         Z VECTOR
       -0.1752591E 00  -0.8727211E-01   0.5055124E-01          -0.4106512E 01  -0.1411451E 01   0.3100037E 01
        0.1292071E 00  -0.6943020E-01   0.1391012E 00           0.1930112E 01  -0.1057861E 01   0.4065296E 01
       -0.2664003E-01   0.1934117E 00   0.5262519E-01          -0.1160014E 01   0.4153644E 01   0.3149157E 01

((((( INSTRUCTION  604 )))))
    0.0           0.0           0.0           0.1540000E 01  0.0           0.0           0.0

     ***** AUTOMATIC SCALE AND POSITION, 50 PERCENT PROBABILITY ELLIPSOIDS **

     ORIGIN POINT IN PLOTTER COORD.(  5.35 ,  5.75 ) IN.
     OVERALL SCALE = 1.960 INCH/ANGSTROM ELLIPSOID SCALE = 1.540
     VIEW DISTANCE 30.000 INCHES
```

```
((((( INSTRUCTION  503 )))))
   0.2000000E 01  0.2700000E 01  0.0            0.0            0.0            0.0            0.0

     ***** STEREO ROTATION OF 2.7 DEGREES ABOUT Y FOR LEFT EYE *****

     ORIGIN FOR PROJECTION AXIS IN CRYSTAL COORD.       0.0            0.0            0.0

     ORTHONORMAL WORKING VECTORS BASED ON CRYSTAL AXES                POST-FACTOR TRANSFORMATION MATRIX
         X VECTOR         Y VECTOR         Z VECTOR
       -0.1726831E 00  -0.8727211E-01   0.5875095E-01           -0.3955544E 01  -0.1411451E 01   0.3290029E 01
        0.1356199E 00  -0.6943828E-01   0.1329401E 00            0.2157155E 01  -0.1057061E 01   0.4768971E 01
       -0.2413946E-01   0.1934117E 00   0.5382206E-01           -0.1010380E 01   0.4153644E 01   0.3200305E 01

((((( INSTRUCTION 1101 )))))
   0.0            0.0            0.0            0.0            0.0            0.0            0.0

     ***** START SAVE SEQUENCE *****

((((( INSTRUCTION  511 )))))
   0.0            0.0            0.0            0.0            0.0            0.0            0.0
     1   4   1   4   4     0.90000     1.60000     0.04000     0.0        0.0        0.0        0.0        0.0

     ***** STORE PROJECTED ATOMS AND BONDS FOR OVERLAP, MARGIN SET BY DEFAULT

     OVERLAP MARGIN IS 0.042 INCH
     CONTENTS OF SORTED ATOMS ARRAY
           455504.   255504.   355504.   355506.   155504.   155506.   355505.   155505.   355502.   155502.
           155503.   155501.   355503.   355501.   255501.   455501.

     BOND SELECTION CODES

     (SEQUENCE(A))(SEQUENCE(B))  (BOND)  (DISTANCES)( BOND )(PERSP.--LABELS)(NORMAL--LABELS)(DIGITS)
     (  MIN   MAX )(  MIN   MAX )  (TYPE)  (MIN    MAX)(RADIUS)(HEIGHT  OFFSET)(HEIGHT  OFFSET)(NUMBER)
          1     4        1     4         4  0.90  1.60   0.040    0.0     0.0      0.0     0.0       0.
     FAULT NO = 14    455504.    800


     BOND OVERLAP ARRAY CONTAINS  19 BONDS (MAXIMUM IS 599)
     ATOM-PAIR NUMBERS IN ARRAY REFER TO SEQUENCE IN SORTED ATOMS ARRAY
             2005.      2006.      2008.      3005.      4006.      5010.      5011.      6010.      6012.      7008.
             8011.      8012.      9010.     10015.     11013.     11015.     12014.     12015.     15016.

     ORIGIN FOR PROJECTION AXIS IN CRYSTAL COORD.       0.0            0.0            0.0

     ORTHONORMAL REFERENCE VECTORS BASED ON CRYSTAL AXES              POST-FACTOR TRANSFORMATION MATRIX
         X VECTOR         Y VECTOR         Z VECTOR
       -0.1752591E 00  -0.8727211E-01   0.5055124E-01           -0.4106512E 01  -0.1411451E 01   0.3108037E 01
        0.1292071E 00  -0.6943828E-01   0.1391012E 00            0.1930112E 01  -0.1057061E 01   0.4065296E 01
       -0.2664803E-01   0.1934117E 00   0.5262519E-01           -0.1160014E 01   0.4153644E 01   0.3149157E 01

((((( INSTRUCTION  715 )))))
   0.4000000E 01  0.0            0.1000000E 01  0.0            0.2000000E 00  0.6000000E 00  0.7000000E 00
   0.0            0.0            0.1000000E 01  0.2000000E 01  0.0            0.0            0.0

     ***** DRAW CARBON ATOM ELLIPSOIDS, ATOM NUMBER RUN 1-2 *****
```

```
((((( INSTRUCTION  712 )))))
      0.0            0.0            0.0            0.0            0.2000000E 00  0.3500000E 00  0.4000000E 00
      0.0            0.0            0.3000000E 01  0.4000000E 01  0.0            0.0            0.0

      ***** DRAW HYDROGEN ATOM SPHERES, ATOM NUMBER RUN 3-4 *****

((((( INSTRUCTION  812 )))))
      0.0            0.0            0.0            0.0            0.0            0.0            0.0
        1  4  1  4  4   0.90000     1.60000     0.04000     0.0        0.0        0.0        0.0        0.0

      ***** TYPE 4 BONDS .04 A MEAN RADIUS, ATOMS 1-4 TO ATOMS 1-4, 0.9-1.6 A

      BOND SELECTION CODES

      (SEQUENCE(A))(SEQUENCE(B)) (BOND) (DISTANCES) ( BOND )(PERSP.--LABELS)(NORMAL--LABELS)(DIGITS)
      (  MIN  MAX )(  MIN  MAX ) (TYPE) (MIN   MAX)(RADIUS)(HEIGHT  OFFSET)(HEIGHT  OFFSET)(NUMBER)
           1    4       1    4        4  0.90  1.60   0.040   0.0     0.0     0.0     0.0       0.
      FAULT NO = 14   455504.   800


((((( INSTRUCTION  906 )))))
      0.1555040E 06  0.1555030E 06  0.0            0.0            0.1500000E 00  0.0            -0.4000000E 00

      ***** LABEL BOND 155504-155503 WITH REGULAR BOND DISTANCE LABEL *****

((((( INSTRUCTION  916 )))))
      0.2555040E 06  0.1555050E 06  0.0            0.0            0.1500000E 00  0.0            -0.4000000E 00

      ***** LABEL BOND 255504-155505 WITH PERSPECTIVE BOND DISTANCE LABEL ****

((((( INSTRUCTION  902 )))))
      0.5555010E 06  0.0            0.0            0.1000000E 01  0.2500000E 00  0.0            0.0

                                            CUBANE

((((( INSTRUCTION 1102 )))))
      0.0            0.0            0.0            0.0            0.0            0.0            0.0

      ***** END OF SAVE SEQUENCE *****

((((( INSTRUCTION  202 )))))
      0.9000000E 01  0.0            0.0            0.0            0.0            0.0            0.0

      ***** ADVANCE PLOTTER 9 INCHES ALONG X *****

((((( INSTRUCTION  503 )))))
      0.2000000E 01 -0.2700000E 01  0.0            0.0            0.0            0.0            0.0

      ***** STEREO ROTATION OF -2.7 DEGREES ABOUT Y FOR RIGHT EYE VIEW *****

      ORIGIN FOR PROJECTION AXIS IN CRYSTAL COORD.       0.0            0.0            0.0

      ORTHONORMAL WORKING VECTORS BASED ON CRYSTAL AXES              POST-FACTOR TRANSFORMATION MATRIX
           X VECTOR        Y VECTOR         Z VECTOR
        -0.1774457E 00  -0.8727211E-01   0.4223930E-01          -0.1240361E 01  -0.1411451E 01   0.2911142E 01
         0.1225073E 00  -0.6943828E-01   0.1451131E 00           0.1698782E 01  -0.1057861E 01   0.4950814E 01
        -0.2909743E-01   0.1934117E 00   0.5131147E-01          -0.1307071E 01   0.4153644E 01   0.3091016E 01
```

```
((((( INSTRUCTION 1103 )))))
      0.0            0.0            0.0            0.0            0.0            0.0            0.0

     ***** EXECUTE SAVED SEQUENCE FOR RIGHT EYE DRAWING *****

((((( INSTRUCTION  511 )))))
      0.0            0.0            0.0            0.0            0.0            0.0            0.0
        1   4   1   4   4    0.90000     1.60000     0.04000     0.0         0.0         0.0         0.0         0.0

     ***** STORE PROJECTED ATOMS AND BONDS FOR OVERLAP, MARGIN SET BY DEFAULT

     OVERLAP MARGIN IS 0.042 INCH

     CONTENTS OF SORTED ATOMS ARRAY
            455504.   355504.   255504.   355506.   155504.   155506.   355505.   355502.   155502.   155505.
            155503.   155501.   355503.   355501.   255501.   455501.

     BOND SELECTION CODES

     (SEQUENCE(A))(SEQUENCE(B)) (BOND) (DISTANCES) ( BOND )(PERSP.--LABELS)(NORMAL--LABELS)(DIGITS)
     (  MIN  MAX )(  MIN  MAX ) (TYPE) (MIN   MAX)(RADIUS)(HEIGHT  OFFSET)(HEIGHT  OFFSET)(NUMBER)
          1    4       1    4        4  0.90  1.60   0.040   0.0     0.0     0.0     0.0      0.
     FAULT NO = 14   455504.   800


     BOND OVERLAP ARRAY CONTAINS  19 BONDS (MAXIMUM IS 599)
     ATOM-PAIR NUMBERS IN ARRAY REFER TO SEQUENCE IN SORTED ATOMS ARRAY
              2005.     3005.     3006.     3010.     4006.     5009.     5011.     6009.     6012.     7010.
              8009.     9015.    10011.    10012.    11013.    11015.    12014.    12015.    15016.

     ORIGIN FOR PROJECTION AXIS IN CRYSTAL COORD.        0.0            0.0            0.0

     ORTHONORMAL REFERENCE VECTORS BASED ON CRYSTAL AXES               POST-FACTOR TRANSFORMATION MATRIX
         X VECTOR          Y VECTOR          Z VECTOR
       -0.1752591E 00  -0.8727211E-01   0.5055124E-01           -0.4106512E 01  -0.1411451E 01   0.3108037E 01
        0.1202071E 00  -0.6943028E-01   0.1391012E 00            0.1930112E 01  -0.1057061E 01   0.4869296E 01
       -0.2664003E-01   0.1934117E 00   0.5262519E-01           -0.1160014E 01   0.4153644E 01   0.3149157E 01

((((( INSTRUCTION  715 )))))
      0.4000000E 01  0.0            0.1000000E 01  0.0            0.2000000E 00  0.6000000E 00  0.7000000E 00
      0.0            0.0            0.1000000E 01  0.2000000E 01  0.0            0.0            0.0

     ***** DRAW CARBON ATOM ELLIPSOIDS, ATOM NUMBER RUN 1-2 *****
((((( INSTRUCTION  712 )))))
      0.0            0.0            0.0            0.0            0.2000000E 00  0.3500000E 00  0.4000000E 00
      0.0            0.0            0.3000000E 01  0.4000000E 01  0.0            0.0            0.0

     ***** DRAW HYDROGEN ATOM SPHERES, ATOM NUMBER RUN 3-4 *****
```

```
((((( INSTRUCTION  812 )))))
       0.0            0.0            0.0            0.0            0.0            0.0            0.0
         1  4  1  4  4    0.90000    1.60000    0.04000    0.0        0.0        0.0        0.0        0.0

      ***** TYPE 4 BONDS .04 A MEAN RADIUS, ATOMS 1-4 TO ATOMS 1-4, 0.9-1.6 A

      BOND SELECTION CODES

      (SEQUENCE(A))(SEQUENCE(B))  (BOND)  (DISTANCES)( BOND )(PERSP.--LABELS)(NORMAL--LABELS)(DIGITS)
      (  MIN  MAX )(  MIN  MAX )  (TYPE)  (MIN   MAX)(RADIUS)(HEIGHT  OFFSET)(HEIGHT  OFFSET)(NUMBER)
           1    4       1    4        4  0.90  1.60   0.040   0.0     0.0     0.0     0.0       0.
      FAULT NO = 14   455504.   800


((((( INSTRUCTION  906 )))))
       0.1555040E 06  0.1555030E 06  0.0            0.0            0.1500000E 00  0.0           -0.4000000E 00

      ***** LABEL BOND 155504-155503 WITH REGULAR BOND DISTANCE LABEL *****

((((( INSTRUCTION  916 )))))
       0.2555040E 06  0.1555050E 06  0.0            0.0            0.1500000E 00  0.0           -0.4000000E 00

      ***** LABEL BOND 255504-155505 WITH PERSPECTIVE BOND DISTANCE LABEL ****

((((( INSTRUCTION  902 )))))
       0.5555010E 06  0.0            0.0            0.1000000E 01  0.2500000E 00  0.0            0.0

                                       CUBANE

((((( INSTRUCTION 1102 )))))
       0.0            0.0            0.0            0.0            0.0            0.0            0.0

      ***** END OF SAVE SEQUENCE *****

((((( INSTRUCTION  202 )))))
       0.2000000E 02  0.0            0.0            0.0            0.0            0.0            0.0

      ***** ADVANCE PLOTTER 20 INCHES *****

((((( INSTRUCTION  402 )))))
       0.0            0.0            0.0            0.0            0.0            0.0            0.0

      ***** ADD DUMMY PLOT TO MAGNETIC TAPE *****

((((( INSTRUCTION   -1 )))))
```

3. DETAILED OPERATING INSTRUCTIONS

3.1 Definitions

Several conventions must be defined before the instructions can be explained.

3.1.1 Atom Designator Code (ADC) and Addressable Point. – In order to specify a particular atom in the crystal within a reasonable distance from the crystallographically defined origin, the following five-component atom designator code word (ADC) is used.

$$ADC = AN*10^5 + (TA + 5)*10^4 + (TB + 5)*10^3 + (TC + 5)*10^2 + SN,$$

where

AN = *ATOM NUMBER* ($0 \leq AN \leq NATOM \leq 166$) the sequential number of the atom in the input list of atoms in the asymmetric unit, which contains NATOM atoms. Atom zero is not in the input atom list but refers to the crystal origin point (0., 0., 0.).

TA, TB, TC *crystal lattice translation digits* along cell edges **a**, **b**, and **c**. Each digit in ADC can range from 1 to 9; consequently, it is possible to move up to ±4 lattice translations in any direction from the origin cell 5,5,5.

SN *symmetry operator number* ($0 \leq SN \leq NSYM \leq 48$) the numerical position of the symmetry operator in the input symmetry operator list which contains NSYM entries. Symmetry operator number zero is not in the input list but refers to an identity operator. However, the identity operation (corresponding to position x, y, z) must in general also be somewhere in the input symmetry operator list and is usually the first operator.

Example: An atom designation code of *347502* refers to atom 3 moved through symmetry operation 2, then translated –1 cell translation along **a**, +2 cell translations along **b**, and 0 cell translations along **c**.

An *addressable point* in the crystal is any point for which an atom designator code exists. In general, the addressable region is approximately a 9 × 9 × 9 block of unit cells.

3.1.2 Vector Designator Code (VDC). – A vector direction is specified by two atom designator codes. The vector direction is from the first to the second.

Example: 253704 263704 is a vector along the positive **a** direction of the crystal lattice.

3.1.3 Atom Designator Run (ADR). – A straight run sequence of atoms can be defined using two atom designator codes with a negative sign preceding the second of the two. The run hierarchy is: first, atom number AN; second, symmetry operation SN; third, **a** translation TA; fourth, **b** translation TB; and last, **c** translation TC.

Example: ADR (145502 –245603) will generate the 8-atom run 145502, 245502, 145503, 245503, 145602, 245602, 145603, 245603.

3.1.4 Atom Number Run (ANR). – The Atom Number Run is a subset of the Atom Designator Run. In this case, only the atom number AN is allowed to change. Normally, an ANR is entered by using only the atom number (AN) values for the first and last members of the sequence without a minus sign.

Example: (1 4) will designate atoms 1, 2, 3, and 4 of the input list.

3.1.5 Vector Search Code (VSC). – A vector search code consists of two atom number runs and a distance range. It is used for finding interatomic distances which have a particular chemical significance, such as covalent and coordination bonds.

Example: Suppose that metal atoms are numbers 1 and 2 in the atom list and oxygen atoms are 6–12 and that the interatomic distance range between metals and oxygens is 1.9 A to 2.4 A. The metal-to-oxygen vectors can be specified by the vector search code (1 2) (6 12) (1.9 2.4). Several variations of this basic code are used in the program.

3.1.6 Sphere of Enclosure. – The sphere of enclosure specifies some or all of the atoms lying within a sphere of radius *D* max about a given "origin" atom without the necessity of delineating each atom individually. This "sphere of enclosure" is said to contain a *complete population* if all addressable atoms within the *D* max radius are included. If the sphere of enclosure contains only certain types of atoms which are derived from a group of sequential atoms in the input list, then the sphere is said to have a *partial population.* Finally, the population (complete or partial) of the sphere of enclosure can be screened as selectively as desired through the use of vector search codes (3.1.5), and the resulting content is called a *vector screened population.*

A sphere of enclosure can be centered on any addressable atom, but one should not use points in the outermost cells as centers because of the possibility of having nonaddressable points within the *D* max radius.

3.1.7 Box of Enclosure. – This is a parallelepiped which can be centered about any addressable point and assigned arbitrary orientation and dimensions. This "box of enclosure" can have a *complete population* or a *partial population* as described for the sphere of enclosure (3.1.6). However, vector screening is not allowed with the box of enclosure.

3.1.8 Reference, Working, and Standard Cartesian Coordinate Systems. – Many of the OR TEP calculations use fractional coordinates based on the crystal axes **a**, **b**, and **c** (triclinic coordinate system); but other steps necessitate the introduction of orthonormal base vector triplets (Cartesian coordinate systems). Two Cartesian systems (reference and working) are utilized. The reference (major) system is used for all operations except plotting, where the working (minor) system is used. For a right-eye or left-eye stereo view, the working system is moved from the reference system by rotation about an axis of the reference system. However, certain decisions made while plotting must still be referred to the reference system to maintain accurate stereopsis. The user can define and orient the two Cartesian systems through the instructions of series 500. Until a 500-series instruction is given, a "standard Cartesian system" is utilized for both the reference and working systems. The orthonormal base vectors of the standard system are oriented as follows:

$$\begin{aligned} &x \text{ axis along } \mathbf{a}, \\ &y \text{ axis along } (\mathbf{a} \times \mathbf{b}) \times \mathbf{a}, \\ &z \text{ axis along } (\mathbf{a} \times \mathbf{b}) \parallel \mathbf{c}^*, \end{aligned}$$

where **a**, **b**, and **c** are crystal axes and $\times$ denotes the outer vector product (cross product). The symbol $\mathbf{c}^*$ refers to a reciprocal axis.

3.1.9 Prime Parameters and Primer Constants. – In the process of mathematically describing an illustration to be machine drawn, many parameters must be used. The more basic among these parameters are called *Prime Parameters*. The values assigned to these prime parameters are often similar or identical from one problem to the next. The first thing OR TEP does is to call subroutine PRIME, which sets as many prime parameters as possible to reasonable, "in the ball park," *Primer Constants*. For example, the maximum plot dimensions (instruction 300 series) are set at 17.0 in. for x maximum and 11.0 in. for y maximum, and the overall scale for plotting (instruction 600 series) is set at 1.0 in. Å. If the value assigned to a particular constant by the primer routine is satisfactory, the user does not have to reset this constant with OR TEP instructions.

3.2 Crystal Structure Data Input

3.2.1 Title Card. – FORMAT (12A6)

Columns	
1–72	Title consisting of any desired alphanumeric identification information. This will appear periodically in the output.

3.2.2 Cell Parameter Card. – FORMAT (6F9.6). Any one of the four following input alternatives may be used (no indicator is needed to specify which type).[1]

Columns	**Type A**	**Type B**	**Type C**	**Type D**
1–9	a (Å)	a (Å)	a^* (Å^{-1})	a^* (Å^{-1})
10–18	b (Å)	b (Å)	b^* (Å^{-1})	b^* (Å^{-1})
19–27	c (Å)	c (Å)	c^* (Å^{-1})	c^* (Å^{-1})
28–36	α (deg)	cos α	α^* (deg)	cos α^*
37–45	β (deg)	cos β	β^* (deg)	cos β^*
46–54	γ (deg)	cos γ	γ^* (deg)	cos γ^*

The parameters a^*, etc., refer to the reciprocal unit cell such that $a \cdot a^*$ 1. All four types will be printed out regardless of which type was used for input.

3.2.3 Symmetry Cards ($1 \leq$ NSYM ≤ 48). – FORMAT (I1,F14.10, 3F3.0,2(F15.10,3F3.0)). The card will be interpreted in one of two ways, depending on the numerical value of the number in columns 70–72. If that number is < 5.0, the card is interpreted as a crystallographic symmetry operation; but if the number is ≥ 5.0, the card is interpreted as a general helix-screw symmetry operation[2] along the c^* crystal axis

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[1] The routine assumes that $a > 1.0$ Å, $a^* < 1.0$ Å^{-1}, α (or α^*) $> 1.0°$, and $|\cos\alpha|$ (or $|\cos\alpha^*|$) < 1.0.

[2] The general helix-screw symmetry operation is not an allowed element of a crystallographic group, so that the molecular environment of the transformed unit will not in general be identical to that of the untransformed unit (unless the crystal is considered to be one dimensional). This input is simply an expedient for use in plotting helical polymer structure models with minimum input. In general it would be possible to produce the same results by specifying the *complete crystallographic asymmetric unit* and normal crystallographic symmetry transformations.

This input mode is only meaningful if the cell angles α and β are 90°, so that c lies along c^* and the helix can continue uninterrupted from cell to cell along the c axis.

(third axis of the standard Cartesian system; see 3.1.8). The two symmetry types can be intermixed if desired.

Columns	(a) Crystallographic symmetry (70–72 ≤ 5)	(b) Helix symmetry (70–72 > 5)
1	≠ 0 last card only	≠ 0 last card only
2–15	T_1	T_1
16–18	S_{11}	–
19–21	S_{12}	–
22–24	S_{13}	–
25–39	T_2	T_2
40–42	S_{21}	–
43–45	S_{22}	–
46–48	S_{23}	–
49–63	T_3	T_3
64–66	S_{31}	L
67–69	S_{32}	M
70–72	S_{33}	N

(a) Crystallographic symmetry[3]: Transformed triclinic coordinates (X_t, Y_t, Z_t) are obtained from input triclinic coordinates (X, Y, Z) by

$$X_t = T_1 + S_{11}X + S_{12}Y + S_{13}Z ,$$
$$Y_t = T_2 + S_{21}X + S_{22}Y + S_{23}Z ,$$
$$Z_t = T_3 + S_{31}X + S_{32}Y + S_{33}Z ,$$

or in matrix notation

$$\mathbf{X}_t = \mathbf{T} + \mathbf{S}\mathbf{X} ,$$

where

$\mathbf{T} = (T_1, T_2, T_3)$ as fractions of cell edges.

(*b*) Helix screw symmetry:

$$\mathbf{X}_t = \mathbf{T} + \mathbf{S}\mathbf{X} ,$$

where

$\mathbf{T} = (T_1, T_2, T_3 + L/N)$ as fractions of cell edge and

$\mathbf{S}$ = a counterclockwise rotation of $L \cdot M/N$ cycles about c* axis.

For example, the Pauling and Corey right-handed alpha helix repeats after 5 turns and 18 residues and can be represented by 18 symmetry cards with $N = 18$; $M = 5$; $L = 0, 1, \ldots, 17$; $T_1, T_2, T_3 = 0$. The input atom list contains the contents of one residue.

3.2.4 Atom Parameter Cards ($1 \le$ NATOM ≤ 166). – Two cards are required for each input atom. The first contains the chemical symbol and positional parameters, and the second contains temperature factor

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[3] Only symmetry cards for *general* symmetry equivalent positions are permitted. Symmetry cards which explicitly designate special positions such as *X, X, X; X, X, Z; X, Y, 0; ½, Y, 0; and ¼, ¼, 0 are not allowed.*

information or other information which specifies how the atom is to be represented on the drawing. The format allows the use of the atom parameter cards produced by the FORTRAN Least Squares Program OR FLS by Busing, Martin, and Levy (1962).[4] Several alternate inputs are possible for each of the two cards, and the number in columns 55–63 denotes the type used on that particular card.

3.2.4.1 Positional Parameter Card. – FORMAT(A6,3X,5F9.6,F9.0)

Columns	Type 0	Type 1	Type 2	Type 3
1–6	Up to six alphanumeric characters centered in the six-place field			
7–9	Blank			
10–18	–	–	–	x_0 (A) Cartesian
19–27	–	–	–	y_0 (A) Cartesian
28–36	x (fractional, crystal)	x (A, crystal)	x (A, Cartesian)	r (A) cylindrical
37–45	y (fractional, crystal)	y (A, crystal)	y (A, Cartesian)	ϕ ( ) cylindrical
46–54	z (fractional, crystal)	z (A, crystal)	z (A, Cartesian)	z (A) cylindrical
55–63	0 or blank	1	2	3

Type 0 is the normal input based on triclinic coordinates. Some authors give coordinates in A along the unit cell vector; type 1 would be used in such a case. Type 2 allows one to place a model described in Cartesian coordinates onto a general triclinic lattice. The orientation of the Cartesian system x y z in the general lattice **a b c** is the standard type described in 3.1.8 with x along **a** and z along **c***. Type 3 is similar to type 2 except that cylindrical coordinates r, ϕ, z are used and the axis of the system can be displaced from zero in the x y Cartesian plane by the displacement x_0, y_0. Cylindrical coordinates are often used in the literature to describe a helical structure. The x_0, y_0 translation should be zero if helical symmetry operators are used. This translation feature is meant to be used in explicitly describing the contents of a multiple helix cell.

3.2.4.2 Temperature Factor Card. – FORMAT(I1,F8.6,5F9.6,F9.0)

Columns	Type 0,1,2,3,10	Type 4,5,8,9	Type 6		Type 7	
1	A sentinel / 0 for last atom only					
2–9	b_{11}	U_{11}	B	B	R	R
10–18	b_{22}	U_{22}	0	0	0	0
19–27	b_{33}	U_{33}	0	$\}\lvert VDC_1\rvert$	0	$\}\lvert VDC_1\rvert$
28–36	b_{12}	U_{12}	0		0	
37–45	b_{13}	U_{13}	0	$\}\lvert VDC_2\rvert$	0	$\}\lvert VDC_2\rvert$
46–54	b_{23}	U_{23}	0		0	
55–63	0,1,2,3,10	4,5,8,9	6 (or 0)	6 (or 0)	7	7

---

[4] W. R. Busing and H. A. Levy, *A Fortran Crystallographic Least-Squares Program*, ORNL-TM-305 (Nov. 21, 1962).

The coefficients b_{ij} $(i,j = 1,2,3)$ of the anisotropic temperature factor, types 0,1,2,3,10, are defined as follows: The complete temperature factor is

$$(\mathrm{Base})^{-D(b_{11}h^2 + b_{22}k^2 + b_{33}l^2 + C\,b_{12}hk + C\,b_{13}hl + C\,b_{23}kl)}$$

where in type 0: Base = e, $C = 2$, $D = 1$,

type 1: Base = e, $C = 1$, $D = 1$,

type 2: Base = 2, $C = 2$, $D = 1$,

type 3: Base = 2, $C = 1$, $D = 1$,

type 10: Base = e, $C = 2$, $D = 2\pi^2$.

The coefficients U_{ij} $(i,j = 1,2,3)$ of the anisotropic temperature factor types 4 and 5 are defined as follows: The complete temperature factor is

$$\exp\left\{ -D\,(a_1^{*2}U_{11}h^2 + a_2^{*2}U_{22}k^2 + a_3^{*2}U_{33}l^2 + Ca_1^*a_2^*U_{12}hk + Ca_1^*a_3^*U_{13}hl + Ca_2^*a_3^*U_{23}kl) \right\} ,$$

where a_1^*, a_2^*, a_3^* are reciprocal cell dimensions and in types 4 and 8, $C = 2$; in types 5 and 9, $C = 1$; in types 4 and 5, $D = \frac{1}{4}$; in types 8 and 9, $D = 2\pi^2$. Type 6 allows the input of the Debye-Waller isotropic temperature factor B, which is used as follows:

$$\exp\,(-B \sin^2 \theta/\lambda^2) ,$$

where λ is the wavelength and θ is the Bragg angle. The parameter B is related to mean-square displacement $\overline{\mu^2}$ of the atom from its mean position by the relation

$$B = 8\pi^2\, \overline{\mu^2} .$$

When the isotropic temperature factor is used, the atom is represented as an isotropic ellipsoid (sphere) with equal principal axes of length μ. When the field in columns 19–27 is 0 or blank, the directions of the principal axes are along the standard Cartesian system axes (see 3.1.8). However, one can reorient these arbitrary orthogonal vectors by using the two vector designator codes VDC_1 and VDC_2; then the three new principal-axis vectors will be VDC_1, $(\mathrm{VDC}_1 \times \mathrm{VDC}_2)$, and $\mathrm{VDC}_1 \times (\mathrm{VDC}_1 \times \mathrm{VDC}_2)$. This is strictly an artistic feature of no physical significance.

Type 7 allows the input of arbitrary spheres of radius $\overline{\mu} = R$ in angstroms. The vector triplet orientation is specified as with type 6. An additional feature allows one to use a completely blank card (except perhaps column 1) for a temperature factor card. In this case the program assumes type 7 with an $R = 0.1$ Å.

A type 10 temperature-factor input card may be used to load Cartesian temperature factors having components in the standard Cartesian system (3.1.8). This feature complements the type 3 Cartesian positional parameter input system (3.2.4.1) and is useful for plotting mean-square displacements caused by internal molecular motions as calculated from spectroscopic normal-coordinate analyses.[5,6]

3.3 Instruction Input

The instructions are the commands used in programming an illustration, and there is no required sequence for the instructions, except as indicated by the programming logic. Some instructions require

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[5] C. K. Johnson, chap. 9 in *Thermal Neutron Diffraction*, ed by B. T. M. Willis, p. 149, Oxford University Press, London, 1970.

[6] R. R. Holmes and R. M. Deiters, *J. Chem. Phys.* **51**, 4043 (1969).

trailer cards, which may have three different formats. The program is informed what the format of the next card will be with the "look ahead" field, columns 1 to 3. The program action is also influenced by this information.

"Look ahead" (columns 1-3)	Next card will be –	Program action
0 or blank	Format No. 0, a new instruction	Execute present instruction; then read next card.
1	Format No. 1, continuation of present instruction	Read continuation card; then check "Look ahead."
2	Format No. 2, vector search code	Read (VSC) card; then check "Look ahead."
3	Format No. 3, alphanumeric info.	Read alphanumeric info. and execute instruction; then read next card.

3.3.1 Instruction Cards. – *3.3.1.1 The Format No. 0 Instruction Card.* – FORMAT(I3,I6,7F9.0)

Columns	
1–3	"Look ahead" (0,1,2,3)
4–9	Instruction number
10–18	1st parameter
19–27	2nd parameter
.	.
.	.
.	.
64–72	7th parameter

3.3.1.2 Format No. 1, Instruction Continuation Card. – FORMAT(I3,I6,7F9.0) A maximum of 19 continuation cards per instruction is permitted.

Columns	
1–3	"Look ahead" (0,1,2,3)
4–9	Blank
10–18	8th parameter, or 15th, . . . , or 134th
.	.
.	.
.	.
64–72	14th parameter, or 21st, . . . , or 140th

3.3.1.3 Format No. 2, Vector Search Code (VSC) Card. – FORMAT(I3,6X,5I3,8F6.0) A maximum of ten VSC cards is allowed. These cards can be entered with any instruction, but only certain instructions will use them. *They must be entered with the particular instructions that require them; that is, they are not held over.* Table 3.1 will be referred to as the individual instructions are explained.

Table 3.1. Vector search code cards

Columns	Search instructions	Inertial axes	Bond plotting instructions			Negative No. in columns 43 to 48	
	101/402 102/412	505/506	801/811/821	802/812/822	803/813	802/812/822	803/813
1–3	Look ahead	Look ahead	Look ahead	Look ahead	Look ahead	Look ahead	Look ahead
4–9	–	–	–	–	–	–	–
10–12	ORG. ANR	ANR	–	ANR (A)	ANR (A)	ANR (A)	ANR (A)
13–15			–				
16–18	TAR. ANR	–	–	ANR (B)	ANR (B)	ANR (B)	ANR (B)
19–21		–	–				
22–24	–	–	Bond type	Bond type	–	Bond type	–
25–30	*D* min (A)	Weight	–	*D* min (A)	*D* min (A)	*D* min (A)	*D* min (A)
31–36	*D* max (A)	–	–	*D* max (A)	*D* max (A)	*D* max (A)	*D* max (A)
37–42	–	–	Bond radius (A)	Bond radius (A)	–	Bond radius (A)	–
43–48	–	–	Perspective label hgt. (in.)	Perspective label hgt. (in.)	–	ANR (P)	ANR (P)
49–54	–	–	Perpendicular displ. (in.)	Perpendicular displ. (in.)	–		
55–60	–	–	Nonperspective label hgt. (in.)	Nonperspective label hgt. (in.)	–	D_p min (A)	D_p min (A)
61–66	–	–	Perpendicular displ. (in.)	Perpendicular displ. (in.)	–	D_p max (A)	D_p max (A)
67–72	–	–	Digits indicator	Digits indicator	–	–	–

3.3.1.4 Format No. 3, Labeling Card. – FORMAT(12A6)

Columns

1–72	Up to 72 digits of alphanumeric label information centered about columns 36 and 37. Note: There is no "look ahead" column in Format No. 3; the next card must be a new instruction card. Instructions 902, 903, and 913 are the only ones which require this input. It may be used with other instructions as a device to transfer comments about the particular instruction to the monitor output listing.

3.3.2 Structure Analysis Instructions (100 Series). – This series of instructions is not connected with drawing illustrations. It is used to obtain on the standard output medium of the computer a convenient tabulation of the chemically interesting aspects of a crystal structure, such as interatomic distances, interatomic angles, and principal axes of thermal motion.

3.3.2.1 Instructions 101 and 102. – These instructions call subroutine SEARCH, which finds all "target" atoms within a sphere of enclosure of radius *D* max about a particular "origin" atom. The instruction card has an atom designator run (see 3.1.3) of origin atoms (Org. ADR) and an atom number run of target atoms (Tar. ANR). The Org. ADR allows one to calculate several spheres successively with a printout of results after each one. For example, suppose there are nine atoms in the input list and we want the total surroundings of atoms 365502, 465502, and 565502 out to a maximum radius, *D* max, of 4 A. The Org. ADR is designated (365502, 5) or (365502, 565502)[7] and the Tar. ANR is designated (1,9). Further selection of the interatomic vectors from a particular origin atom to the target atoms which fall within the limiting sphere is possible with vector search code (VSC) cards of Format No. 2 (see 3.3.1), which can be entered with the instruction. If VSC cards are present, then the vectors must also satisfy one of the VSC's in order to be saved. A VSC card to specify the selection of a shell of vectors in the above example might be coded as follows: Org. ADR (3,5) Tar. ANR (1,9) Dist. range (2.0, 2.7). More selective VSC's are also possible. They are meant to be based on known interatomic distance ranges, such as those tabulated in Vol. III of the *International Tables for X-Ray Crystallography.*[8]

Vectors found about a particular origin atom are stored in a table of dimension 200 sorted on distance. Duplicate vectors (not duplicate distances) are eliminated. If more than 200 acceptable atoms are found about an origin atom, the 200 shortest vectors are saved. At the end of the search about each origin atom, the distances are printed out along with the atom designator codes (ADC), chemical symbols, and triclinic crystal coordinates for the origin and target atoms. If the instruction is 102, all possible interatomic angles and interatomic distances for the edges opposite the angles are also calculated and printed for the stored vectors. There will be $n(n-1)/2$ angles for n vectors.

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[7] For the origin sequence 355501, 455501, 555501, an Org. ADR input (3,5) is allowed as well as (355501,5) and (355501,555501); however, the Tar. ANR must always be designated as shown. In sect. 2.1, Org. ADR is designated as ORG 1, ORG 2; and Tar. ANR is denoted by TAR 1, TAR 2. A minus sign preceeding the second member of the Org. ADR is not required.

[8] H. Ondik and D. Smith, "Interatomic Distances in Inorganic Compounds," p. 257 in *International Tables for X-Ray Crystallography,* vol. III, ed. by K. Lonsdale, Kynoch, Birmingham, 1962.

The tabulation of atom designator codes, which is obtained automatically when these instructions are given, is often useful for planning an illustration. Although the tabulation is complete within the addressable region of 9^3 cells, the computing time is generally only a matter of seconds per sphere unless a very large *D* max is specified. Subroutine SEARCH is a rather elaborate routine designed to minimize computing time. This subroutine is also used for instructions 402 and 403, which are explained in 3.3.5.

Instruction card for instructions 101 and 102:

Columns	
1–3	0 or 2 (look ahead)
4–9	101 or 102
10–18	Origin-ADR (atom designator run)
19–27	
28–36	Target ANR (atom number run)
37–45	
46–54	D max (A)

3.3.2.2 Instruction 103. – Principal axes of thermal motion (or arbitrary spheres, according to the temperature factor input) for all atoms in the input list are calculated. The printout contains root-mean-square amplitudes of displacement along the principal axes of the trivariate normal probability density function and direction cosines for the principal axes relative to the reference Cartesian base vectors. A symmetric covariance dispersion matrix based on the reference Cartesian system is also printed out. The diagonal elements are the mean-square displacements along the reference Cartesian axes.

Columns	
1–3	0 or blank (look ahead)
3–9	103
10–18	Blank

3.3.2.3 Instructions 105 and 106, Convoluting Sphere of Enclosure and Reiterative Convoluting Sphere of Enclosure. – These instructions utilize the ATOMS table and can only be used after one or more atoms have been placed in the table by a 401, 402, 403, or 404 instruction. The contents of the table are returned to the condition of entry at the conclusion of instructions 105 and 106.

All atoms in the ATOMS table which have atom numbers within the origin atom number run (Org. ANR) of the instruction are used as origin points. Interatomic distances for all neighboring atoms (whether or not in the ATOMS table) are found out to the specified radius. Vector-search-code (VSC) cards may be used for screening if desired.

Instructions 105 and 106 are similar, except that instruction 106 keeps repeating the "convolution" process until no new atoms with atom numbers within the Org. ANR are found.

Instruction 106 is useful for molecular structures where the atoms in the input asymmetric unit do not form an intact molecule. In a case of this nature, it is advisable to place a single atom into the ATOMS table with a 401 instruction and let a 106 instruction find the molecule. Care must be taken to specify a D max which will enclose only bonded atoms. The 106 instruction should *not* be used for structures forming infinite chains.

Columns	
1–3	0 or 2 (look ahead)
4–9	105 or 106
10–18	Origin ANR (atom number run)
19–27	
28–36	Target ANR (atom number run)
37–45	
46–54	D max (A)

3.3.3 **Plotter Control Instructions (200 Series).** – The 200 series is a group of instructions that control the plotter initialization, frame advance, termination, and any other peripheral commands that are required for a particular equipment configuration or plotting package. When the program is modified for a different equipment configuration, these series 200 instructions, which are executed through subroutine F200, should be redefined to suit the user's requirements. Instructions for controlling the CalComp 765 and 835 off-line magnetic tape plotting systems[9] are given here.

3.3.3.1 Instruction 201. Plot Package Initialization. Mechanical Plotter. – This instruction (or a 203 instruction) must be executed before any plotting can take place. It is a safe policy always to make this the first instruction card. It should be used only once per computer job regardless of how many plots are to be drawn during the job. If the 201 (203) and 301 instructions are omitted, all calculations are carried out but no plotting is done.

3.3.3.2 Instruction 202, Plot Terminate and Frame Advance. – This takes care of putting the correct plot termination information onto the magnetic tape to inform the plotter that the current plot is finished. It also allows advance of the paper so that the old plot is removed and new paper is in position for the next plot.

Columns	Instruction 201	Instruction 202
1–3	Blank	Blank
4–9	201	202
10–18	–	Plotter movement along x edge of paper in inches

---

[9] The CalComp is an incremental plotter. The particular Benson-Lehner model available at Oak Ridge Central Data Processing Facility has also been used. The Benson-Lehner is an electromechanical x-y plotter with an analog converter. In general it seems that an incremental plotter is better suited to the requirement of ORTEP. The user should be warned that in the author's experience the magnetic tape plotting systems are notoriously troublesome; an annoying percentage of plot failures is to be expected because of equipment malfunctions. (This was true in 1965 and is still true in 1975.)

3.3.3.3 Control Instructions for CalComp Model 835 Cathode-Ray-Tube Plotter. – In order to plot interchangeably on the CRT and the mechanical CalComp plotters, an extended 200 series of instructions is necessary.

A 203 instruction initializes the CRT plotter and is used in place of the 201 instruction. In general, no other changes are needed except that the plotting area specified by the 301 instruction must not exceed 17 in. in x and 11 in. in y. (The 301 primer constants are set accordingly.)

Columns		
1–3	Blank	
4–9	203	
10–18	XORG	(new position of the origin of plotter coordinates relative to the lower left-hand corner of the normal CRT plotting area)
19–27	YORG	
28–36	IZORG (beam intensity origin)	

The entries for XORG, YORG, and IZORG are normally zero or blank.

The beam intensity, IZ, can be changed from its initialized value IZ = IZORG + 18 to any other value in the range 0 to 30 with a 204 instruction. The usable range of IZ is about 12 to 24 with the higher values producing darker lines.

Columns	
1–3	Blank
4–9	204
10–18	IZ – IZORG

The frame advance instruction 202 is interpreted differently for CRT usage; however, the same 202 instruction cards used for a mechanical plotter plot can also be used for a CRT plot. Any positive number in columns 10 to 18 of the 202 instruction (3.3.3.2) will add a block address (i.e., plot number) to the magnetic tape and will advance the film to a new frame. A value of zero in columns 10 to 18 will add a block address but will not advance the film to a new frame, and a negative value will terminate the output magnetic tape file. It is not normally necessary to use the negative value option since the termination is taken care of automatically when the -1 instruction is executed if a 201 instruction was not executed after the 203 initialization instruction; however, if the mechanical plotter is to be used during the same job, the negative value option allows the CRT to be terminated properly before initialization of the mechanical plotter.

3.3.4 Plot Boundary Instructions (300 Series). – This is a set of miscellaneous instructions for specifying the dimensions of the drawing, viewing distance, general lettering orientation, and pen displacement for line retracing.

3.3.4.1 Instruction 301. – This instruction defines the limiting x and y dimensions, in inches, of the plot boundary and the border indentations. The boundary dimensions must not exceed those allowed by the plotter. The program will prevent the pen from getting closer than 0.1 in. to any boundary. The border indentation is an equal margin inside the entire boundary. When automatic scaling is used (600 series), the center points of the atoms are prevented from falling in the margin; but the atom representation, which has a finite size, may extend into that area. To compensate for the overlap, the border dimensions should be large when the overall drawing scale and the ellipsoid scale are expected to be large.

In addition, instruction 301 specifies the perspective viewing distance, in inches, from the plane of the drawing. An entry of 0 for view distance is used to indicate an infinite view distance, and the crystal structure is then mapped in parallel projection normal to the drawing board.

Columns		Primer Constant
1–3	–	–
4–9	301	–
10–18	Plot x limit (in inches)	17.
19–27	Plot y limit (in inches)	11.
28–36	View distance (in inches)	0. (parallel proj.)
37–45	Border (in inches)	0.5

3.3.4.2 Instruction 302, Title Rotation. – For regular titles and chemical symbols, the title rotation is specified with instruction 302. The lettering base line for all lettering is rotated counterclockwise by an angle theta, in degrees, from the x axis of the plotter. Although any value is allowed, 0° and –90° are the values most often used, so that, when one views the finished drawing, either the y plotter axis is vertical or the x plotter axis is vertical.

Columns		Primer Constant
1–3	Blank	–
4–9	302	–
10–18	Theta in degrees	0.

3.3.4.3 Instruction 303, Retrace Displacement. – For artistic purposes, certain lines are made heavier than others by retracing over the path several times with slight pen displacements (DISP) from the original path. For example, in drawing ellipsoids the forward half of the principal plane trace is made heavier than the hidden half so the eye does not confuse the two halves. In addition all regular lettering (but not perspective lettering) is gone over four times to give it boldface appearance. In preliminary runs or when the plotter is not of the incremental type, this embellishment may be objectionable to the user because of the increased computing and plotting times (particularly the latter). All retracing can be eliminated by setting DISP = 0. The primer parameter for DISP is 0.005 in., which is the resolution of the CalComp plotters at ORNL. For other plotters or for various inking pen sizes, DISP can be reset at the user's discretion. Retracing should not be used with a CRT plotting device.

Columns		Primer Constant
1–3	–	–
4–9	303	–
10–18	DISP (in inches)	0.005

3.3.5 Atom List Instructions (400 Series). – This series allows the user to specify which atoms are to be included in the illustration. The atom designators for the chosen atoms are stored in the ATOMS array for future use by other instructions. The ATOMS array can hold 500 atoms; but if the intended illustration has more than this, the illustration can be segmented and the segments drawn sequentially on the same plot.

Groups of atoms are added to or eliminated from the ATOMS array (which is set to zero at the start of the program) with the 400 and 410 series respectively. The groups can be denoted by atom designator runs (see 3.1.3), spheres of atoms about any center point (see 3.1.6), and boxes of atoms centered on any point (see 3.1.7). Duplicate entries of the same atomic position are prevented by the program. The content of the ATOMS list is printed on the monitor output tape after each 400 series instruction.

3.3.5.1 Instructions 401 and 411, Atom Designator Run Add and Atom Designator Run Eliminate. – These instructions can contain: (*a*) atom designator codes (ADC) for a single atom, (*b*) atom designator runs (ADR) for several atoms in a run, (*c*) blank fields (except between the two entries of a run), and (*d*) any combinations of (*a*), (*b*), and (*c*). Since up to 19 Format No. 1 continuations are possible per instruction, up to 70 runs can be made per instruction and an unlimited number of instructions can be used. The ATOMS list, however, will only accept the first 500 atoms.

Columns	
1–3	Blank or 1 (depending on what follows)
4–9	401 or 411
10–18 . . . 64–72	As described above

3.3.5.2 Instructions 402 and 412, Sphere of Enclosure Add and Sphere of Enclosure Eliminate. – These instructions allow the user to build or modify the subject by specifying the contents (complete, partial, or vector screened, see 3.1.6) of a sphere of enclosure about any addressable point. For instruction 402, the contents of the spheres are *added to* the atom list except for positional duplications, which are omitted. In the 412 instructions, all points in the spheres are *eliminated from* the atoms list if they are present in that list. The instructions call subroutine SEARCH, and the instruction input details are identical to those of instructions 101 and 102 (see 3.3.2.1) except for the instruction number. In the monitor output, only the ATOMS list atom designator codes are printed and not the coordinates and interatomic distances. If the origin atoms on which the spheres of enclosure are centered are to be saved, the target atom number run (Tar. ANR) must contain this atom number. Furthermore, if vector search code cards of Format No. 2 are used, one of them must satisfy the intra-atom null vector for the origin atom in order to retain it.

3.3.5.3 Instructions 403 and 413, Box of Enclosure Add and Box of Enclosure Eliminate. – These instructions allow the user to build or modify the subject by specifying the contents (complete or partial but *not* vector screened, see 3.1.7) of a box of enclosure about any addressable point (or atom designator run of addressable points). The three axes of the box are parallel to the three base vectors of the reference Cartesian system, and the *semidimensions* of the box are specified on the instruction card. If an orientation of the box different from the standard orientation (see 3.1.8) is desired, than a 501 or a 502 instruction, or both, should be used before this instruction to reorient the reference Cartesian system. After this instruction has been executed, the reference system can undergo further reorientation as desired for plotting purposes, etc.

As in the case of the sphere of enclosure (see 3.3.5.2), the origin atom on which the box is centered will not be included unless the target atom number run includes the origin atom number. Vector search codes are not used by this instruction. Subroutine SEARCH is used by this instruction, and the instruction input details are similar to those described in 3.3.2.1 except that *D* max is replaced by the semidimension *a*/2 of the box and the following fields on the card are used to specify the other two semidimensions *b*/2 and *c*/2. One must use caution in choosing the box dimensions so that the atom table does not overflow.

Columns	
1–3	Blank
6–9	403 (or 413)
10–18 19–27	Origin ADR (see 3.3.2.1)
28–36 37–45	Target ANR (see 3.3.2.1)
46–54	*a*/2 (A)
55–63	*b*/2 (A)
64–72	*c*/2 (A)

3.3.5.4 Instructions 404 and 414, Triclinic Box of Enclosure Add and Triclinic Box of Enclosure Eliminate. – These instructions are similar to instructions 403 and 413, except that the triclinic box of enclosure is bounded by planes parallel to the principal planes of the crystal lattice. The semidimensions *a*/2, *b*/2, *c*/2 refer to fractional (triclinic) coordinates. To specify the contents of the conventional unit cell, one would use *a*/2 = *b*/2 = *c*/2 = .5, and the Org. ADR would refer to a point in the input atom list at 1/2, 1/2, 1/2.

3.3.5.5 Instructions 405, 406, 415, 416; Convoluting Sphere of Enclosure Add, Reiterative Convoluting Sphere of Enclosure Add, Convoluting Sphere of Enclosure Eliminate, and Reiterative Convoluting Sphere of Enclosure Eliminate. – These instructions are used in the same manner as instructions 105 and 106 (see 3.3.2.3). Their function is to add atoms to or eliminate atoms from the ATOMS table. A valid origin atom must be placed in the ATOMS list with a 401, 402, 403, or 404 instruction before the present instructions are used. All atoms in the ATOMS table which have atom numbers within the origin atom number run (Org. ANR) of the instruction are used as origin points of convolution.

An important use for the 405 instruction is to complete the coordination shells around metal atoms without having to describe any of the atoms individually. Another use might be to obtain a cluster of atoms out to the *n*th neighbor when only the distance to the first neighbor is known. This can be accomplished by using *n* consecutive 405 instructions with D max slightly more than the first neighbor distance.

Instruction 406 is useful for describing molecular compounds when an unfortunate choice of atoms for the input asymmetric unit does not allow the molecule to be described by a run. D max must be chosen judiciously so that the search does not cross molecular boundaries.

The input format is identical to that described in 3.3.2.3, with the appropriate instruction number in columns 4–9.

3.3.5.6 Option for Examining E-Map Results – Stereoscopic drawings are useful for the rapid screening of *E* maps when direct methods are used for solving crystal structures. First the interpolated positions of the largest peaks in the Fourier synthesis *E* map are punched on cards directly by a Fourier program. Then OR TEP starts at a given peak (usually the largest) and does a reiterative-sphere-of-enclosure-add instruction (406) to isolate a molecule if one is present. In order to terminate the convolution procedure when extraneous "bridging peaks" link the molecules, a modification was added to the 406 instruction which allows an atom (in any of its equivalent positions) to be entered in the ATOMS list only once. To invoke this feature, a type 1 continuation card (3.3.1.2) with a 1 in column 18 is added to the 406 instruction. The 406 instruction operates normally if the continuation card is omitted (3.3.5.5).

3.3.5.7 Instruction 410. Clear Atoms List. – This instruction clears the atoms list to zero. When the program is first entered, the list is automatically set to zero.

3.3.6 Orienting Instructions (500 Series). – This series of instructions orients the reference and working Cartesian systems (see 3.1.8). Each time the reference system is redefined with a 501 or rotated with a 502, the working system is automatically made coincident with the reference system. The working system can be displaced from the reference system by rotating about an axis of the reference system with a 503 instruction. The working system is always positioned by a rotation from the reference system and does not depend on the previous working system orientation. After each 500 series instruction, the base vectors of the relevant Cartesian system are printed out. These vectors are based on the triclinic coordinate system. The postfactor transformation matrix for converting from triclinic coordinates to Cartesian coordinates is also printed out. The inverse transformation matrix may be formed by placing the three base vectors together in row vector form.

3.3.6.1 Instruction 501, Reference Cartesian System Assignment. – Any Cartesian coordinate system is based on three orthonormal base vectors and an origin point. The origin point in the model (ORGN) is specified with an atom designator code. The three orthonormal base vectors can be described by two noncollinear vectors, and OR TEP provides the two following separate techniques for performing this operation, using vector cross products of the two vectors **u** and **v**.

	Type A	Type B
Base vector 1 (x axis)	$\mathbf{u}$	$\mathbf{u}$
Base vector 2 (y axis)	$\mathbf{u} \cdot \mathbf{v}$	$(\mathbf{u} \cdot \mathbf{v}) \cdot \mathbf{u}$
Base vector 3 (z axis)	$\mathbf{u} \cdot (\mathbf{u} \cdot \mathbf{v})$	$\mathbf{u} \cdot \mathbf{v}$

The reference system x and y axes will parallel the plotter x and y axes, and the origin point ORGN will lie in the plane of the plotter. The viewer will be looking into the z axis vector of the coordinate system from a distance VIEW in inches (see 3.3.4.1) directly above the origin point.

Columns		Effective Primer Constant
1–3	–	–
6–9	501	–
10–18	Origin (ADC)	000000
19–27	Vector $\mathbf{u}$ (VDC)	155501
28–36		165501
37–45	Vector $\mathbf{v}$ (VDC)	155501
46–54		156501
55–63	–	–
64–72	0 = Type A, >0 = Type B	1

3.3.6.2 Instruction 502, Reference Cartesian System Rotation. – The crystal model can be given any orientation desired with a series of rotations of the model about the reference system axes. In general, three rotations (e.g., those of an Eulerian system) are sufficient to achieve any orientation, but for convenience an unlimited number of rotations are permitted in the program. In addition, rotations of 120° about the body diagonal of the reference Cartesian system are permitted (this is achieved by a cyclic permutation of reference base vectors).

Each operation requires two fields in the instruction card. For axial rotations, the first field of each pair will have the number 1, 2, or 3 to indicate rotation about the x, y, or z axes of the reference system. The second field will have the rotation angle in degrees for a right-handed rotation of the model about the designated axis (i.e., a positive angle signifies a counterclockwise rotation of the structure with the designated axis pointing toward the reader). The body diagonal rotation is designated by either a (– 1) or a (– 2) in the first field to indicate a 120° or a 240° right-handed rotation about the body diagonal, and the second field is blank. A (– 3) would rotate the structure completely around and thus not change its previous orientation.

Columns	
	First Card
1–3	0 (or 1 if continued on next card)
4–9	502
10–18	1,2,3,–1,–2
19–27	ϕ_1
28–36	1,2,3,–1,–2
37–45	ϕ_2
46–54	1,2,3,–1,–2
55–63	ϕ_3
64–72	1,2,3,–1,–2
	Second Card
10–18	ϕ_4
.	
.	
.	

If desired, each rotation can be executed with a separate 502 instruction card.

3.3.6.3 Instruction 503, Working Cartesian System Rotation (Stereoscopic Rotation). – The working (minor) Cartesian system is automatically made coincident with the reference system whenever the reference system is redefined with a 501 instruction or rotated with a 502 instruction. To define an orientation of the working system which is not coincident with the reference system we use a 503 instruction, which allows one rotation about one axis of the reference system. Actually any number of successive rotations can be made, but the effect is not cumulative since the starting point for each rotation is always the reference system. Body diagonal rotations are not permitted.

A 503 rotation normally precedes each member of a stereoscopic pair of plots. The rotation is about axis 2 if the stereo pair is to be viewed with the x axis parallel to the observer's interocular line and about axis 1 if the y axis is to be parallel to that line.

Columns	
1–3	–
4–9	503
10–18	1,2,3
19–27	[illegible]

3.3.6.4 Optimal Parameters for Stereoscopic Drawings. – Figure 3.1 shows a geometrical construction which may be used to derive the parameters used in making stereoscopic drawings.[10,11] The empirical parameters in common usage [(*a*) 30-in. view distance, (*b*) 5 to 6 stereo rotation, and

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[10] J. T. Rule, *J. Opt. Soc. Am.* **28**, 313 (1938).

[11] B. G. Saunders, *Appl. Opt.* **7**, 1499(1968).

(c) a photographic reduction to achieve 2.2 to 2.4 in. separation of equivalent points) produce quite satisfactory results with a slightly exaggerated impression of depth. Theoretically, the best stereoscopic fidelity is obtained by translation of the origin rather than by stereo rotation of the object.[11] however, the comparison of results given in Fig. 3.2 shows that the differences are indeed minor and nearly impossible to detect. Stereo by translation of origin is achieved with instruction 504, which may be used in place of the 503 instruction, however, the 504 instructions should not be used when the ellipsoids have internal structure because the octants selected for shading may not be the same on both stereo views.

Columns	
1–3	Blank
4–9	504
10–18	Translation of origin along x axis of reference system (in.)
19–27	Translation of origin along y axis of reference system (in.)
28–36	Translation of origin along z axis of reference system (in.)

For the geometrical conditions depicted in Fig. 3.1, the stereo-rotation instructions for the left and right eyes,

503 2 2.45

and

503 2 −2.45 ,

are replaced by the stereo translation instructions

504 −1.28 0 0

and

504 2.56 0 0 ,

respectively. If additional drawings are to be made, the origin first should be returned to its original position with the instruction

504 −1.28 0 0 .

in order to prevent confusion.

3.3.6.5 *Instruction 505. Origin at Centroid.* – This instruction finds the first moment (i.e., centroid or center of gravity) of the atoms in the ATOMS list and makes this point the ORIGIN of the reference and working coordinate systems. A weighting scheme and screening may be applied to the atoms by using format No. 2 trailer cards (see Table 3.1). If no trailer cards are used, all atom positions are entered with unit weights.

3.3.6.6 *Instruction 506. Origin at Centroid and Inertial Axis Coordinate System.* – The calculation described for instruction 505 is performed, then the second moment matrix about the centroid is calculated, and the reference and working coordinate systems are set up along the principal axes of this matrix. This principal axis system of coordinates is along the inertial axis of the configuration of atoms in the ATOMS list. The x axis is along the long axis of the configuration (i.e., the minimum axis of inertia) and the z axis is along the short axis of the configuration (i.e. the maximal axis of inertia). The overlap

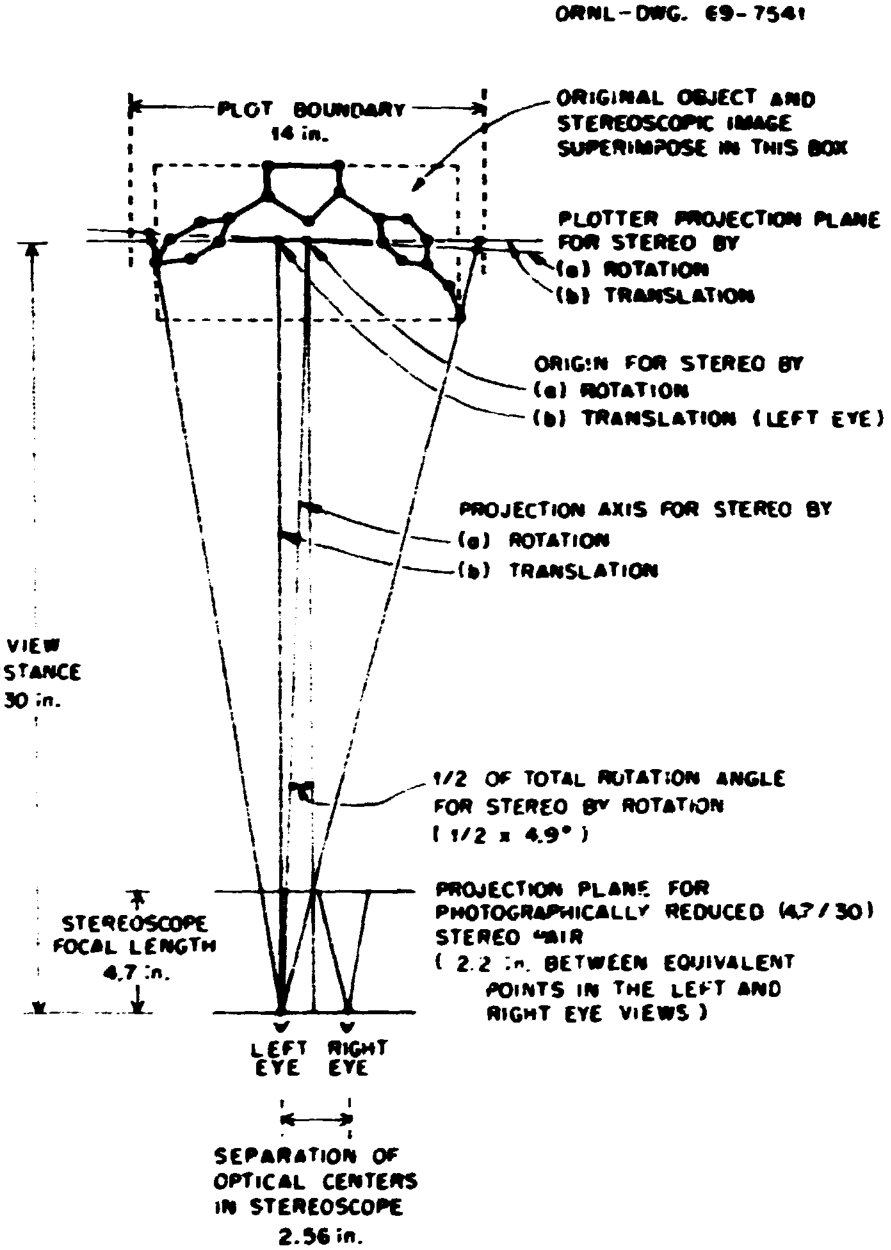

Fig. 3.1. Geometrical Relations Among the Stereoscopic Perspective Projection Parameters for a Typical OR TEP Drawing. The available plotting area for each projection is assumed to be 14 in. horizontally and at least 11 in. vertically. The scaled mathematical object is within a box 12 in. wide, 9 in. (or more) high, and 6 in. deep with the plane of the plotter halfway back into the box. The stereoscopic image seen through a stereoscope with a 12-cm (4.7-in.) focal length and a 6.5-cm (2.56-in.) separation between optical centers should appear superimposed on the original object. The parameters for both "translation stereo" and "rotation stereo" are shown. The appropriate linear dimensions can be scaled to accommodate other plotting areas and still produce the same final image.

ORNL DWG. 69-8122

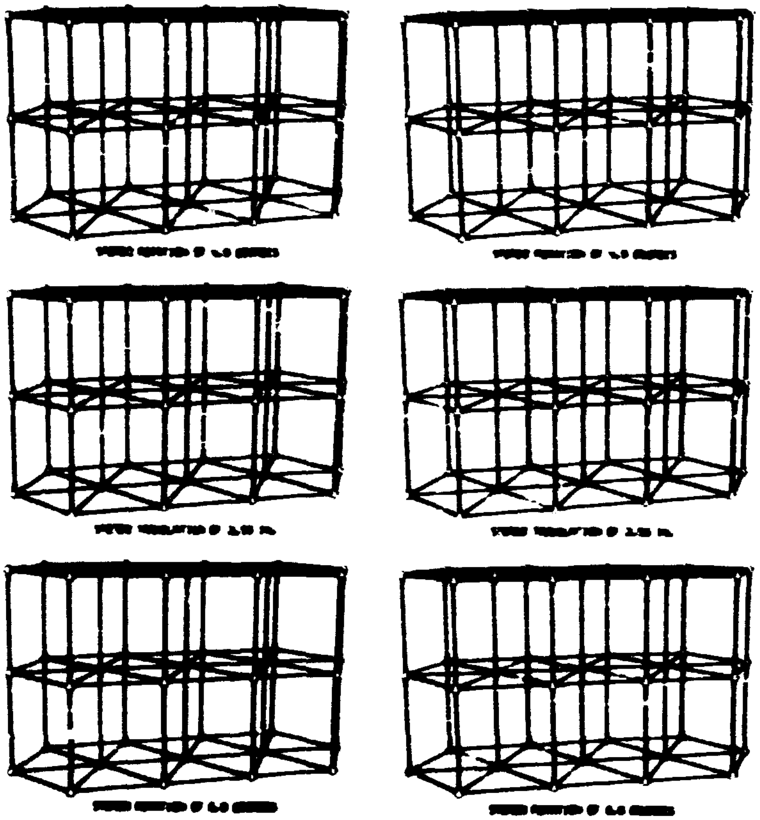

Fig. 3.2. Three Stereoscopic Drawings of a Hexagonal Lattice with Different Stereoscopic Parameters. The top and middle drawings utilize the parameters derived in Fig. 3.1 and demonstrate that the differences predicted (ref. 11) for translation and rotation stereo are not discernible in practice. The bottom stereo drawing illustrates the slight exaggeration in depth which occurs when a larger stereo rotation angle is used. The drawings should be viewed individually with a 12-cm focal-length stereoscope of good optical quality.

along the z-view direction is often minimized by this option. Furthermore, the x-y plane is the least-squares best plane for the atomic configuration. Format No. 2 trailer cards may be used to supply weights and screening (see Table 3.1).

3.3.6.7 Instruction 511. Overlap Elimination. – See Section 3.3.14.

3.3.7 Positioning and Scaling Instructions (600 Series). – These instructions are used to direct the placement of the origin point ORGN (specified by instruction 501) onto the drawing (dimensioned by instruction 301). In addition the three-dimensional assembly of atoms (chosen by the 400 series instruction) constituting the model is scaled. The atomic centers of the model will then be hanging in space above and below the drawing board correctly positioned to be projected from the eye point described with 301.

3.3.7.1 Normal Modes of Positioning and Scaling. – Several normal modes of operation are available to the user for positioning and scaling the model. Instruction 601 requires the user to supply a complete explicit description of position (x_0, y_0) and scale (SCAL1). At the other extreme, instruction 604 automatically scales and positions the model so that the peripheral projected atom centers will touch two opposite borders and the peripheral atoms in the remaining dimensions will be centered on the drawing. An intermediate mode is available through 602, which provides automatic scaling after explicit positioning. In general this allows only one edge of the model to touch a border. Finally, instruction 603 requires an explicit scale and does automatic centering.

In general the 604 instruction is the easiest and safest one to use, but situations arise in which the user should not relinquish control to the program. For example, if a big illustration is to be drawn piecewise on a small plotter, the user will have to maintain control over the scale, and probably over positioning, so that the partial plots can be fitted together correctly.

A second scale factor SCAL2 is required in connection with the ellipsoid (or sphere) size. It is a dimensionless scale factor ratio used to modify all rms displacement values before plotting equiprobability ellipsoids or spheres. A table of SCAL2 values vs probability is given in Sect. 5.2. The primer constant for SCAL2 is 1.54, corresponding to 50% probability. If the instruction's entry for SCAL2 is 0 or blank, then SCAL2 is not modified by the instruction. The same statement also holds for x_o, y_o, and SCAL1. That is, if the instruction entry is zero or blank for any of these, then the value of the constant in memory is not changed. This means that an x_o or y_o cannot be entered as exactly zero, so that if zero is wanted, a small nonzero number should be entered.

Columns	601	602	603	604	Primer Constant
1–3	–	–	–	–	–
4–9	601	602	603	604	–
10–18	x_o	x_o	–	–	8.5
19–27	y_o	y_o	–	–	5.5
28–36	SCAL1	–	SCAL1	–	1.0
37–45	SCAL2	SCAL2	SCAL2	SCAL2	1.54

3.3.7.2 Incremental Modes of Positioning and Scaling. – Additional flexibility is provided through the incremental instructions 611, 612, and 613. These allow the user to "nudge" the model or modify the scale factor (SCAL1), or both, after the parameters have been initially set with a previous 600 series instruction. The 611 instruction adds Δx_o, Δy_o to the previous x_o, y_o position for the ORGN placement and multiplies the existing SCAL1 by ΔK (except if $\Delta K = 0$, SCAL1 is unmodified). Instruction 612 increments the position and then does an automatic scaling; 613 first increments the scale (by multiplying by ΔK) and then automatically repositions.

A conservative general approach is to follow a 604 with a 611 having $\Delta x_o = 0$, $\Delta y_o = 0$ and $\Delta K = 0.9$. This will simply reduce the scale 10% so that there is more space for labels, etc.

Column	611	612	613
1–3	–	–	–
4–9	611	612	613
10–18	Δx_0	Δx_0	–
19–27	Δy_0	Δy_0	–
28–36	ΔK	–	ΔK
37–45	SCAL2	SCAL2	SCAL2

3.3.8 Atom Plotting Instructions (700 Series). – These instructions are concerned with drawing various representations of the atom based on the familiar ball-and-stick molecular model. The ball in the general case is an ellipsoid representing a contour surface of equal probability density. Alternatively, when thermal motion is not being portrayed, the ball can be a sphere of arbitrary dimension. The 700 series also has provision for labeling the atomic site with the corresponding chemical symbol. The instructions in this series draw the "ATOMS list" atoms which project onto the usable part of the drawing area. Atoms found to be out of bounds are bypassed, and a Fault Message (NG = 10) is printed on the monitor output. An atom is out of bounds under the following conditions: (1) if its z coordinate in the scaled reference Cartesian system is greater than $\frac{1}{2}$ the viewing distance, (2) if its center after projection falls outside the limiting boundary of the drawing board, or (3) if the projected center is within $\frac{3}{4}$ of the margin width (BRDR) of a limiting boundary.

An ellipsoid, for graphical purposes in OR TEP, is considered to be composed of ellipses and straight lines. The ellipses are of two types, principal ellipses and boundary ellipses. Relative to the viewpoint, a principal ellipse is further subdivided into a front half and a back, or hidden, half. There are three principal ellipses per ellipsoid, corresponding to the three principal planes. The boundary ellipse is the edge of the ellipsoid as seen from the viewpont. The front and back halves of the principal ellipses meet at the boundary ellipse. The straight-line segments of the OR TEP ellipsoid are the forward principal axes, reverse principal axes, and octant shading lines.

Figure 3.3 shows various combinations of these elements. It is obvious that certain of these combinations are better representations than others. Instruction 701 generates the 5A model of Fig. 3.3, instruction 702 generates 2A, and 703 produces 3B. Instruction 704 draws the boundary ellipse alone. If an atom is entered as a sphere, the boundary will be circular before projection and slightly elliptical after perspective projection. Instruction 705 allows the user to make up any representation from the basic components.

Chemical symbols up to six alphanumeric characters in length are included with the input structural parameters for each atom. These symbols can be put onto the illustration with one 700 series or several 900 series instructions. The 700 series places the center of the six-character field of each atom in the same position relative to the atom center; the 900 series allows the user to position each symbol individually. The 700 series requires only three parameters as follows: (1) symbol height in inches, (2) parallel (left-right) offset in inches, and (3) perpendicular (up-down) offset in inches. The parameters refer to the model before projection, and they will change slightly during perspective projection. The parallel and

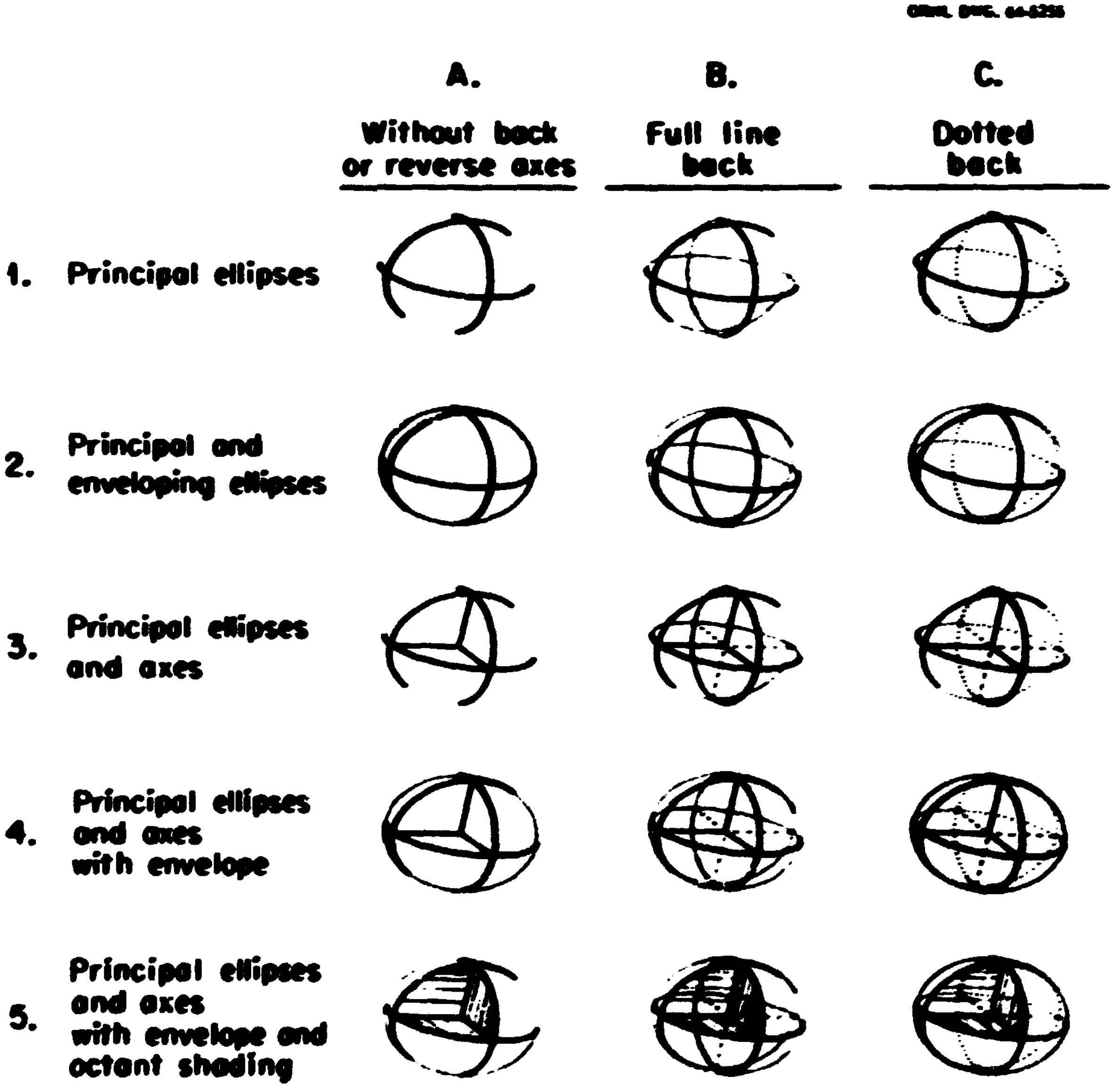

Fig. 23. Various Combinations of Ellipsoid Components.

perpendicular offset refer to the exact center of the six-character input field and are relative to the lettering base line set up with the 302 theta rotation. A symbol height of 0 or blank will cause the symbol-drawing routine to be bypassed.

In order to distinguish certain atoms, such as those in disordered positions, a 705/715 instruction with NPLANE = 4, NDOT = 3, 4, 5, or 6, NLINE = 0, and NDASH = 0 may be used to produce dotted boundary ellipses to contrast with the normal solid line boundary ellipses. Another feature of the 705/715 instruction is that if NPLANE = 0, and if the symbol height is greater than zero, then chemical symbols alone are drawn on the atomic sites.

It is possible to vary the thickness of the boundary ellipse line by making it a function of z, the height of the atom from the drawing board. This option is normally used with the 704 (boundary only) instruction but will work for any 700 instruction. Entries are put in the A_0 and A_1 fields of the instruction continuation card to specify the coefficients of

$$\Delta R(z) = A_0 + A_1 z ,$$

where

ΔR is the increase in radial dimension to be added to the width of the single pen line,

A_0 is ΔR for an atom at $z = 0$, and

A_1 is the rate of increase in radial dimension with z.

As an example, assume that the atoms of the scaled model range from 5 in. below to 5 in. above the drawing board and the pen width is 0.2 mm (.008 in.). If we want the closest ellipse boundary to be five times as wide as the farthest, then $\Delta R(-5 \text{ in.}) = 0$, $\Delta R(5) = 0.008 \times (5 - 1) = 0.032$ in.; thus $A_0 = 0.016$ in. and $A_1 = 0.0032$ in.

The program widens the line by stepping radially in increments of DISP, which is set by primer constant to 0.005 in. A 303 instruction can be used to change DISP if desired.

Selected types of atoms from the ATOMS table can be drawn without having to alter the contents of the table. This is accomplished by using an atom-number-run (ANR) code which includes the atom types that are to be drawn with a particular 700-series instruction. This feature is particularly useful when two or more different representations are used such as for the carbon and hydrogen atoms in the cubane example. If no ANR is entered, then all atoms in the table are drawn.

The monitor output for the 701 through 705 instructions consists of the following:

1. x,y plotter coordinates: the coordinates, in inches, for the projected atom center on the plot, measured from the lower left-hand corner of the limiting boundary. This is the fixed plotter coordinate system with origin point set by the plotter operator.

2. x,y,z working Cartesian coordinates: the coordinates, in inches, for the oriented and scaled atomic model before projection. The x and y axes parallel the plotter x and y axes, and the origin of the system is in the plane of the plotter at the point x_0,y_0 (see 3.3.7) in plotter coordinates. The point ORGN of the scaled model is at this point (see 3.3.6.1).

3. x,y,z triclinic coordinates, in fractions of the unit-cell edges relative to the crystal unit-cell origin.

4. Principal axes of thermal motion, consisting of (*a*) principal values of root-mean-square displacement and (*b*) direction cosine for principal vectors relative to the working Cartesian system.

5. The atom designator code and chemical symbol for the atom.

Instructions 711 through 715 are identical to 701 through 705 except that *the 710 series suppresses all monitor output except fault messages.*

3.3.8.1 Atom Plotting Instructions 701, 702, 703, 704, and 711, 712, 713, 714. –

Columns	
	First Card
1–3	1 (if boundary retracing or atom selection is desired; otherwise 0)
4–9	701, 702, 703, 704, 711, 712, 713, 714
10–45	Blank
46–54	Symbol height (in.)
55–63	Parallel offset (in.)
64–72	Perpendicular offset (in.)
	Second Card (needed only for boundary retracing or atom selection)
1–3	Blank
4–9	Blank
10–18	A_0 (in.) or blank
19–27	A_1 (in.) or blank
28–36 37–45	AKR or blank

3.3.8.2 Atom Plotting Instructions 705 and 715. –

Columns		
	First Card	
1–3	1 (if boundary retracing or atom selection is desired; otherwise 0)	
4–9	705 or 715	
10–18	NPLANE = 0, no ellipsoid components = 1, boundary ellipse only = 3, principal ellipses only = 4, boundary + principal ellipses	
19–27	NDOT (back side of principal ellipses) < 0, solid line back side = 0, back side omitted = 3, 4 dots on back side = 4, 8 dots on back side = 5, 16 dots on back side = 6, 32 dots on back side	
28–36	NLINE (forward principal axes and shading) = 0, no forward axes or shading = 1, forward principal axes only = N, forward axes + (N – 1) line shading	
37–45	NDASH (dashed reverse principal axes) = 0, no reverse axes = N, dashed reverse axes with N dashes	
46–54	Symbol height (in.)	
55–63	Parallel offset (in.)	for symbols
64–72	Perpendicular offset (in.)	
	Second Card same as 701	

3.3.9 Bond Plotting Instructions (800 Series). – The bond plotting instructions are grouped into two general types, explicit and implicit, depending on how the bonds are specified. Explicit bonds require a vector designator code (see 3.1.2) for each bond. Implicit bonds make use of vector search codes (see 3.1.5) to find pairs of atoms from the ATOMS array set up by the 400 series instructions.

There are two types of bonds that can be drawn, stick bonds and line bonds. The line bond is a very crude, but rapid, method useful in drawing preliminary illustrations. It is constructed by placing centered symbols (e.g., +, x, *, etc.) on the two atom sites and drawing a single straight line between them. Line bonds are always specified implicitly (803, 813 instructions).

The more elaborate bond is the stick bond, which could also be called a conical bond because of its accentuated perspective taper.[12] Each end of the bond intersects either (1) an ellipsoid or (2) an enveloping cone (tangent cone) which has its apex at the viewpoint and is tangent to an ellipsoid. In general, the ellipsoid intersection is automatically used if the axis of the bond intersects the ellipsoid at a point which is visible to the viewpoint; otherwise, the tangent cone intersection is used, so that the bond appears to terminate at the boundary of the ellipsoid. However, the user can specify that the ellipsoid intersection always be used in order to make the skeleton type model (e.g., 3B of Fig. 3.1) appear even more transparent. The radius of the stick bond and the number of lines which are used to draw the bond are specified by input parameters.

Bond-distance labels can be drawn automatically with stick bonds, but not with line bonds. The bond-distance label numbers are in Angstrom units to one, two, or three places past the decimal point. The bond labels on the illustration will have their base lines parallel to the stick bonds and will be right side up for the viewer. The height of the label in inches and the perpendicular offset distance for the center of the label relative to the center of the bond are parameters to be specified by the user. With the present primer constant for FORE, if the sine of the angle between the bond and the mean viewing vector is greater than 0.5, the lettering is done in perspective along the bond. When the sine of the angle is less than 0.5, the perspective lettering would be excessively foreshortened; the lettering is then made parallel to the plane of the drawing with its base line parallel to the projected bond. Different lettering heights and different perpendicular offset distances can be assigned to the perspective and nonperspective bond-distance labels.

All bond parameters are input with Format No. 2 trailer cards (see 3.3.1). The bond parameters are as follows:

1. Bond type (for stick bond) is designated by an integer NBOND, where $-5 \le \text{NBOND} \le 5$. The negative integers denote that both ends of the bonds terminate at the ellipsoids. The positive integers denote bonds ending either at the ellipsoid or the tangent cone, as described previously in this section. An entry of zero draws no bond. A magnitude of 1 for NBOND produces two lines, one for each bond edge, 180° apart in the plane normal to the bond axis. Lines are drawn 90°, 45°, 22.5°, or 11.25° apart for NBOND magnitudes of 2, 3, 4, or 5, respectively. The back side of the bond is not drawn. Representative samples are shown in Fig 6.1.

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[12] The accentuated taper may be increased or decreased by changing the value assigned to TAPER in SUBROUTINE PRIME (see TAPER in sect. 4.5).

2. The bond radius (mean value for stick bonds) is in Angstrom units. Values between 0.01 and 0.06 A usually give good results. Any positive value may be used as long as it is smaller than the scaled ellipsoid minimum semidimension. The bond radius is not changed by the ellipsoid scale factor ratio SCAL2. The bond radius should not be made "vanishingly small" (e.g., $r < 0.005$ A) if the overlap feature is used because numerical rounding may cause incorrect hidden-line elimination.

3. The height of perspective labels for bond distances is entered as zero if no bond distances are to be labeled. Positive values denote the lettering height in inches before projection.

4. The perpendicular offset for bond distance perspective labels (in inches) pertains to offset of the center of the distance label relative to the center of the bond.

5. The height of regular labels for bond distances is entered as zero if no bond distances corresponding to foreshortened bonds are to be drawn. Positive values give the lettering height in inches before projection.

6. The perpendicular offset for bond-distance regular labels has the same definition as parameter 4 above.

7. The significant digits indicator is −1, 0, or 1, denoting bond distance labels with one, two, or three digits, respectively, after the decimal place.

The use of vector-search-code (VSC) cards for the bond plotting instructions 802 and 803 has been extended to include a provision for drawing coordination polyhedra while suppressing the unwanted bonds. In addition to describing the bond with ANR(A), ANR(B), and the D min to D max range, a condition can be imposed to require that both atoms must be within a specified "polyhedral distance range" of an atom in the ATOMS table which has an atom number satisfying a third atom number run, ANR(P). This option is brought into play by a negative number in columns 43 to 48 of the VSC card and is applicable to instructions 802, 803, 812, and 813.

Instructions 801, 802, and 803 differ from 811, 812, and 813 only in the monitor output listing. The second group has no output except error messages. The first group lists: (1) plotter coordinates in inches, (2) scaled Cartesian coordinates (in inches) of atom before projection, and (3) triclinic crystal coordinates for the atoms of each bond. The interatomic bond distance in angstroms is also listed. If an atom of a bonded pair is out of bounds, a fault message (NG = 10) is printed on the monitor output. If the bond is hidden and cannot be drawn, fault message NG = 14 is printed. Fault NG = 13 signifies that an imaginary intersection was found with a bond radius larger than the ellipsoid semidimension.

3.3.9.1 Instructions 801 and 811, Explicit Stick Bonds. – The bonds are described with two atom designator codes for each bond. The atom designator codes go on the 801 card and on Format No. 1 trailer cards (see Table 2.1 for format). The two atom designator codes for a bond must be in adjacent fields, but blank fields can be inserted between the different bonds. Since there are seven fields available per card, it is a good idea to use only two, four, or six of them so that the card sequence within the instruction (other than first and last cards) will be unimportant. In addition, a Format No. 2 trailer card is required with the fields specified under column 801 in Table 3.1 properly filled in.

3.3.9.2 Instructions 802 and 812, Implicit Stick Bonds. – All parameters are input with Format No. 2 trailer cards (see Table 3.1). The only entry on the instruction card is the instruction number and look ahead (2).

3.3.9.3 Instructions 803 and 813, Implicit Line Bonds. – All parameters are input with Format No. 2 trailer cards (see Table 3.1). The centered symbol placed on a given atom will be the centered symbol whose calling number corresponds to the atom number modulo 10 (see Fig. 4.2).

The centered symbols drawn on the atomic sites by the 803–813 instructions may be made larger or smaller by redefining the SCAL2 factor, which is controlled by the 600 series of instructions (3.3.7).

3.3.9.4 Instructions 821 and 822, Overlap Elimination. See Section 3.3.14.

3.3.10 Label Plotting Instructions (900 Series). – The 900 series allows the user to plot general titles up to 72 characters in length, chemical symbols up to 6 characters long, bond length labels, and centered symbols. The bond length labels can have two decimal places before the decimal point and one, two, or three places after the decimal point. The 700 and 800 series instructions can plot chemical symbols and bond length labels, but it is often desirable to position certain labels individually with the 900 series.

General titles and bond length labels can be drawn either in perspective or parallel to the plane of the drawing. Chemical symbols and centered symbols are always drawn parallel to the plotter plane. Instructions 913 through 916 are for perspective lettering, and instructions 901 through 909 produce regular lettering.

Two vectors, the upright vector and the base-line vector, are needed to describe a lettering plane. In OR TEP the upright lettering vector is always parallel to the plane of the drawing. For perspective lettering the base-line vector is a general vector in three dimensions. In the nonperspective case the base-line vector is either along the projection of a general vector or along the vector (in the plane of the plotter) which is oriented with a 302 title rotation instruction (theta base line). If theta (set by 302) is zero, then the theta base-line vector is along the plotter positive *x* axis.

The exact center of the label is always referred to when specifying the position of the label. The program goes through the following steps to position the center point of the label onto the drawing. (1) A point *P*1 is found which is either the position of atom A or the mean of two atom positions (atom A and atom B). The atom A position is used if no atom designator exists in the atom B field of the instruction card. (2) A point *P*2 is found by (*a*) translating from *P*1 along the base-line vector for the distance specified by *parallel offset*, then (*b*) translating along the upright vector by the *perpendicular offset* distance. (3) A point *P*3 is found by projecting *P*2 onto the plane of the plotter. (4) If the *x edge reset* is >0, then *x* is reset to this value. If *x edge reset* is < 0, *x* is reset to the positive *x* plot boundary minus |*x edge reset*|. No resetting is done if *x edge reset* is zero. The *y* parameter is handled in the same manner with *y edge reset*.

The format for the entire 900 series is as follows:

Columns	
1–3	Blank or 3 (or 1 if second card is needed)
4–9	Instruction number
10–18	Designator for atom A
19–27	Designator for atom B (or blank)
28–36	x edge reset (in.)
37–45	y edge reset (in.)
46–54	Lettering height (in.)
55–63	Parallel offset (in.)
64–72	Perpendicular offset (in.)
	Second Card (if needed)
1–3	Blank
4–9	Blank
10–18	Centered symbol number (0–14)

3.3.10.1 Instruction 901. – A nonperspective chemical symbol with theta base line is drawn using the chemical symbol for atom A.

3.3.10.2 Instruction 902. – A nonperspective title with theta base line is drawn. The title must be entered with the instructions on a Format No. 3 trailer card. The title should be centered about columns 36–37 of that card.

3.3.10.3 Instructions 903 and 913. – A general vector title is drawn with nonperspective lettering for 903 and perspective lettering for 913. The general vector is from atom A to atom B. The title is entered as described for 902 (see 3.3.10.2 above).

3.3.10.4 Instructions 904, 905, 906, 914, 915, and 916. – These are instructions for general-vector bond-length labels. The first three are for nonperspective lettering with one, two, and three places after the decimal point; and the last three are for the corresponding bond-length labels with perspective lettering. The general vector is from atom A to atom B. Note that the sense of the vector is important in order to have the label right side up.

3.3.10.5 Instructions 908 and 909. – These instructions are for centered symbols. With 908 the pen is up while moving to the position where the centered symbol is to be drawn, but ***with 909 the pen is left down.*** The centered symbol is one of the 15 listed for the CalComp SIMBOL routine (the misspelling of "symbol" is intentional). The symbol number must be in the range 0–14.

3.3.11 Saved Sequence Instructions (1100 Series). – It is often desirable to repeat a sequence of instructions one or more times with other instructions inserted between the repetitions. The 1100 series allows the user to do this without the necessity of putting in duplicate sequences of instruction cards. It is not an elaborate looping device, but it does give additional flexibility to the system.

The three instructions in this series are to start the saved sequence (instruction 1101), terminate the saved sequence (instruction 1102), and execute the saved sequence (instruction 1103). All instruction cards and their trailer cards between the 1101 and 1102 instructions are executed and saved on a magnetic scratch tape. A 1103 instruction rewinds this scratch tape and repeats all the instructions stored there before another instruction is read from the monitor input. There are no parameters to be entered with the 1100 series instructions.

3.3.12 Job Termination Instructions (Negative Series). – A (–1) instruction terminates the job and exits via SUBROUTINE EXIT.

A (–2) instruction reinitializes the whole program and starts over with another structure from the title card on. As many structures as desired may be run in sequence in this manner before exiting with a (–1) instruction. Note that the 201 instructions should occur only once and should not be repeated for succeeding jobs.

3.3.13 Supplementary Instructions (1200 Series). – These instructions utilize Subroutine SPARE.

3.3.13.1 Punching Cards with OR FLS Format. – An instruction 1201, which is implemented in subroutine SPARE, punches new position cards and temperature-factor cards with the format used by the OR FLS least-squares program. The instruction is useful for transforming a structure to a different asymmetric unit and for saving key atoms from a complex ATOMS array. First an ATOMS array is generated by the 400 series of instructions; then positional parameter cards, taken from the input atoms list, are read to define which atoms are wanted and to supply information about the scattering factor identifier and the multiplier. The parameter cards for all atoms in the ATOMS list which are crystallographically equivalent to the ones read are punched out. The sequence of the parameter cards read by this instruction need not correspond with the sequence of the original input atoms.

Columns	
1–3	Blank
4–9	1201
10–18	*n* (the number of positional parameter cards to be read: *n* position parameter cards from the original input atom deck must follow this instruction card.)

3.3.14 Overlap Correction Instructions (511, 821, 822). – The hidden line correction feature of OR TEP-II eliminates most of the manual touch-up tasks previously required to correct for overlapping atoms and bonds. Drawings made with the overlap feature activated may require up to two or three times the computing time needed for noncorrected drawings; consequently, it is often more economical in computer time to make the preliminary drawings without overlap correction, particularly if a large number of atoms are present in the drawing.

To utilize the overlap feature an additional instruction, 511, is required, which is usually accompanied by type 2 trailer cards identical to those used by the 802 or 812 instructions. The 511 instruction stores the projected atom boundary ellipses for all atoms in the ATOMS list. It is important that the contents of the ATOMS list, the scaling and positioning, and the viewing parameters (controlled by the 400, 600, and 500 series of instructions respectively) not be changed between the 511 instruction and the drawing of the atoms and bonds by the 700 and 800 series of instruction; otherwise, the projected outlines may be destroyed or may be inappropriate.

The projected bond outlines, approximated as quadrangles, also may be stored for the overlap correction either by adding format No. 2 trailer cards to the 511 instruction or by using one or more 822 instructions (including those format No. 2 trailer cards) after the 511 instruction. The bonds to be stored are specified implicitly by the format No. 2 trailer cards. Explicit bonds also may be stored by using an 821 instruction (after the 511 instruction) with parameters identical to the 801/811 instructions to be used for plotting the explicit bonds.

The projected outline information for atoms and bonds must be recalculated for each member of a stereo pair, consequently the 511 and 821 or 822 instructions are usually the first instructions within the saved sequence. The old overlap information is removed whenever a new 500 or 600 series instruction is executed.

The maximum number of projected atoms and projected bonds which can be stored is 500 and 599 respectively. A list of the projected atoms and bonds is given in the printout.

An important feature of the OR TEP-II scheme for correcting overlap is that all details *inside* atoms and bonds, including chemical symbols and bond-distance labels, will be corrected for overlap, however, note that chemical symbols (drawn by the 700 series instructions and bond-distance labels (drawn by the 800 series instructions) which are *outside* the atoms or bond boundary *may not be corrected* for overlap. The reason for this is that the "area overlap search step" does not save projected atoms or bonds which do not contact the projected atom or bond to be drawn. Labels or symbols drawn with the 900 series instructions will not be corrected for overlap.

3.3.14.1 *Instruction 511. Projected Outline Storage.* – A constant width overlap margin (i.e., a blank strip at the intersection of overlapping elements) is included in the dimensions of each projected atom ellipse and projected bond quadrangle. The width of this margin may be specified as a parameter with the 511 instruction if desired; otherwise, the margin is set by default to either 0.025 inch or $(\mathrm{SCAL1})^{1/2} \cdot 0.030$ inch, whichever is largest. Some users prefer an overlap margin of 0.0 for stereoscopic drawings.

Columns	
1–3	2 (if bonds are to be stored, otherwise 0)
4–9	511
10–18	Blank or 0 – overlap margin default option described above 1 (or –1) – overlap margin = 0.0 0 < OVMRGN ≤ 1.0 – overlap margin = OVMRGN (in inches)

If column 3 is 2, format no. 2 trailer cards are included. In general all the trailer cards included with the 802/812 instructions are used.

3.3.14.2 *Instruction 821. Explicit Bond Outline Storage.* – If explicit bonds are to be stored for the overlap calculation, the attached atoms must be in the ATOMS list even though this is not a requirement for the 801/811 instructions used for plotting the explicit bonds. See 3.3.9.1 (Instructions 801 and 811) and Table 3.1 for description of parameters.

3.3.14.3 Instruction 822. Implicit Bond Outline Storage. – Normally the information on implicit bond outlines is stored with the 511 card; however, if more than 10 Format No. 2 trailer cards are needed, the extra ones can be entered with this instruction. All parameters are entered with the Format No. 2 trailer cards (see Table 3.1). The only entry on the instruction card is the 2 in column 3 and 822 in columns 7–9.

3.4 List of Fault Indicators

Certain errors are checked for in OR TEP, and when one of these occurs, an error message, "FAULT NG *ng ADC m*" is written on the monitor output tape. The number NG is explained below. The *ADC* and *m* identify the atom code and the instruction involved (if these are relevant). If possible, corrective measures are made by OR TEP and the calculation proceeds; otherwise, the job is terminated by calling SUBROUTINE EXIT.

NG	Subroutine Involved	Fault	Action
1	PRELIM	No sentinel found after reading 48 symmetry cards	Tries to read parameter cards
2	PRELIM	No sentinel found after reading the parameter cards for 100 atoms	Tries to read instruction cards
3	PRELIM	Anisotropic temperature factor coefficients form a matrix which is not positive definite	EXIT after printing out all rms principal values (imaginary ones are listed negative)
4	ATOM,PAXES	Symmetry operation number is higher than the number of input operations	Omit atom
5	ATOM,PAXES	Atom number is higher than the number of input atoms	Omit atom
6	EIGEN	Null temperature factor matrix or failure in bisection routine	EXIT, after printing out all principal values
7	EIGEN	Eigenvector routine failure due to null vector	EXIT, after printing out all principal values
9	MAIN,SPARE	Unidentified instruction number	Omit faulty instruction
10	BOND,F700	Atom out of bounds	Omit atom
11	F800	No vector search codes	Omit instruction
12	F600, SEARCH	Insufficient number of atoms in ATOMS list	EXIT
13	BOND	Imaginary bond intersection (i.e., bond larger than atom)	Omit bond
14	BOND	Hidden (end-on) bond	Omit bond
15	F900	Null vector as base line	Omit label
16	STORE	ATOMS list is full	Omit all succeeding atoms

4. COMPUTATIONAL PROCEDURES (HOW THE PROGRAM WORKS)

Certain of the numerical procedures[1] used in OR TEP are of a nature somewhat unfamiliar to many crystallographers. These aspects are outlined for the benefit of the reader who may wish to write a similar program or modify the present one.

4.1 Graphic-Computational Methods

These are the techniques used in producing the graphical details of the illustrations.

4.1.1 Drawing Ellipsoids. – Figure 3.1 demonstrates the various ellipsoid graphical representations that can be drawn with OR TEP. The major components in the representations are the three principal ellipses and the boundary (outline) ellipse. The principal ellipses have a front half and a back (hidden) half. The entire boundary ellipse is visible.

An ellipse is approximated by connecting a series of points on the ellipse with straight line segments. Points on an ellipse having a general orientation in three dimensions are computed; then each of these points is projected onto the drawing board for plotting.

The basic algorithm for finding the points along a given general ellipse utilizes the properties of conjugate diameters. Assume that we have the three principal axis vectors **V1**, **V2**, **V3** of the general ellipsoid and a vector **V4** from the center of the ellipsoid to the viewpoint. The vector **V5** normal to the polar plane (see Fig. 4.1), whose pole is the viewpoint, can be obtained from

$$\mathbf{V5} = \mathbf{A}\mathbf{V4}\,. \qquad (4.1.1.1)$$

where **A** is the matrix for the ellipsoid which is defined by

$$\mathbf{X}^T\mathbf{A}\mathbf{X} = d\,. \qquad (4.1.1.2)$$

where d is a constant.

The boundary ellipse is defined by two conjugate vectors, one of which is any vector **V6** perpendicular to **V5** and the second is **V7**, where

$$\mathbf{V7} = \mathbf{V5} \times \mathbf{A}\mathbf{V6}\,. \qquad (4.1.1.3)$$

The assumption made for this boundary ellipse derivation is that the view distance is large compared to the ellipsoid size. Therefore, the boundary ellipse defined above always lies on the diametral polar plane (see Fig. 4.1).

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[1] For a treatment of the projective and analytical geometry involved, the following four books are recommended. The first one is particularly useful.

J. Heading, *Matrix Theory for Physicists*, chap. 3, pp. 81-106, Longmans, Green and Co., London, 1958.

C. E. Springer, *Geometry and Analysis of Projective Spaces*, Freeman and Co., San Francisco, 1964.

J. A. Todd, *Projective and Analytical Geometry*, Pitman Pub. Corp., New York, 1946.

G. A. Korn and T. M. Korn, *Mathematical Handbook for Scientists and Engineers*, McGraw-Hill Book Company New York, 1961.

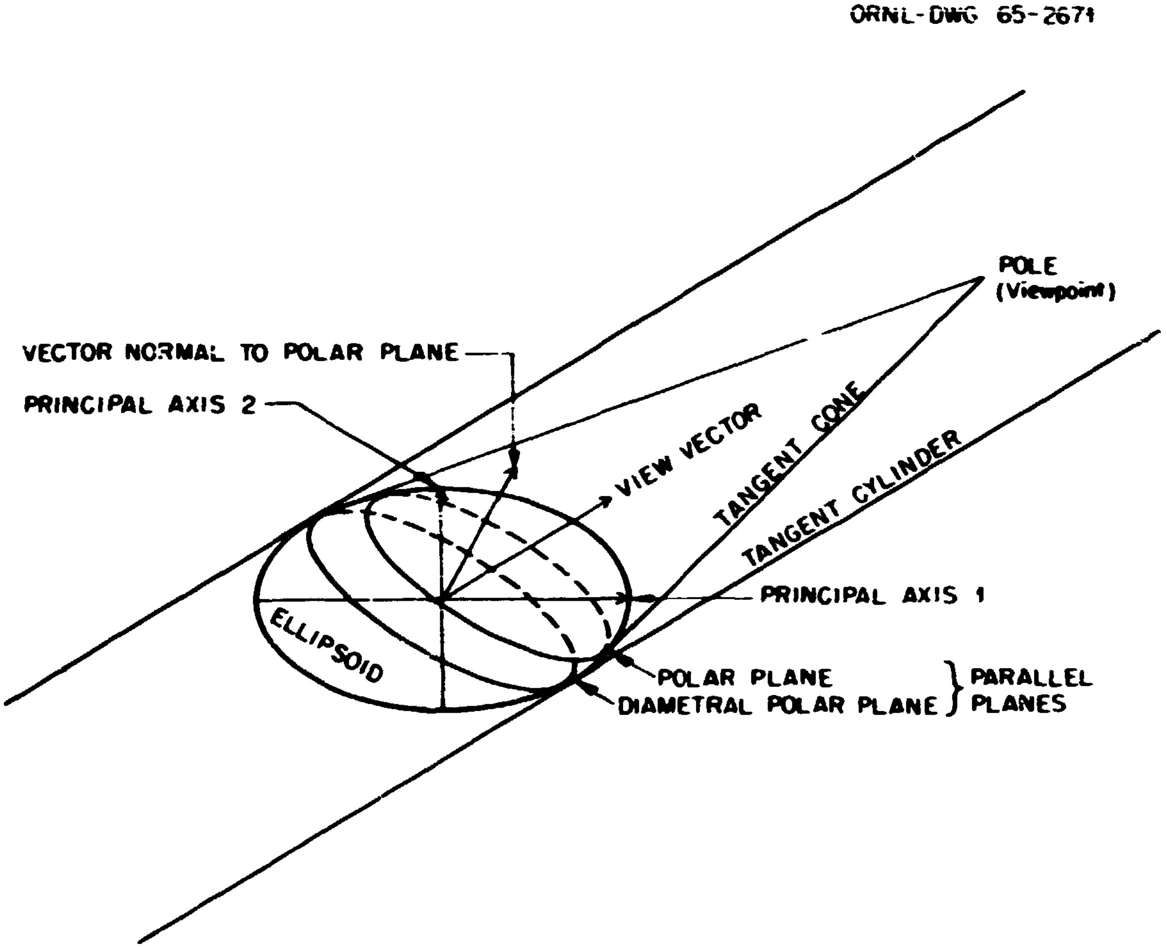

Fig. 4.1. Polar Planes Formed by Tangent Cylinder and Tangent Cone.

A principal ellipse which lies in the plane of the principal axis vectors **V1** and **V2** will have the third principal axis vector **V3** normal to the plane of the ellipse. The intersection of this principal ellipse with the boundary ellipse is along the vector **V8** where

$$\mathbf{V8} = \mathbf{V5} \times \mathbf{V3} \,. \tag{4.1.1.4}$$

This vector divides the front and back (hidden) sides of the principal ellipse. A vector conjugate to **V8** and in the principal plane containing **V1** and **V2** is **V9**, where

$$\mathbf{V9} = \mathbf{V3} \times \mathbf{A}\,\mathbf{V8} \,. \tag{4.1.1.5}$$

After the conjugate vectors have been found, their lengths are adjusted to make them satisfy (4.1.1.2) by letting $\mathbf{X} = s\,\mathbf{l}$ where $\mathbf{l}$ is a unit vector. Solving for s, we obtain

$$s = [d/(\mathbf{l}^T \mathbf{A}\,\mathbf{l})]^{1/2} \,. \tag{4.1.1.6}$$

A conjugate vector pair is expanded into an ellipse by subroutine RADIAL. Since an ellipse is centrosymmetric, the two conjugate vectors and their negatives give us four vectors whose end points lie on the ellipse. By performing a vector sum of two adjacent vectors and dividing the resultant vector components by $\sqrt{2}$, we can obtain an additional vector. After doing this for all adjacent pairs, we then have a total of eight vectors. This process can be repeated as many times as desired except that the scaling constant will be different for each cycle. The constant is described by

$$\mathrm{CONT}\,(i) = \{2[1 + \cos(\pi/2^i)]\}^{1/2} = 2\cos(\pi/2^{i+1})$$

where i is the cycle number.

This total process may be thought of as taking a planar radial set of equally spaced unit vectors and performing a deformation and scaling on the space in which it is described. In geometry this deformation is called an affine transformation.

Complete details on drawing ellipsoids can be obtained from the FORTRAN coding of subroutines F700 and RADIAL.

4.1.2 Drawing Bonds. – The major problem in drawing bonds is to obtain the intersection where the bond penetrates the ellipsoid. Three quadrics are used in subroutine BOND to calculate bond intersection. These three are the ellipsoid, the tangent cylinder, and the tangent cone.

The ellipsoid is described in matrix notation as

$$\mathbf{X}^T \mathbf{A} \mathbf{X} = d\,, \tag{4.1.2.1}$$

where d is a constant and $\mathbf{X}$ is any vector from the center to the surface of the ellipsoid. The matrix $\mathbf{A}$ is 3 by 3 symmetrical with components a_{ij} $(i,j = 1, 2, 3)$.

The elliptic cylinder tangent to the ellipsoid and with its axis along z is described by

$$\mathbf{X}^T \mathbf{B} \mathbf{X} = d\,, \tag{4.1.2.2}$$

where

$$\mathbf{B} = \begin{pmatrix} a_{11} - \dfrac{a_{13}a_{31}}{a_{33}} & a_{12} - \dfrac{a_{23}a_{31}}{a_{33}} & 0 \\ a_{12} - \dfrac{a_{13}a_{32}}{a_{33}} & a_{22} - \dfrac{a_{23}a_{32}}{a_{33}} & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{4.1.2.3}$$

and d is the constant used in (4.1.2.1). The tangent cylinder is used when it is necessary to terminate the bond at the boundary of the ellipsoid *when a parallel projection is used.*

To find the intersection of a cylindrical bond along $\mathbf{Vb}$ with radius r with either the ellipsoid or the tangent cylinder, we proceed as follows:

1. Form a radial set of vectors $\mathbf{Vr}_i$ of length r normal to $\mathbf{Vb}$.

2. Take a unit vector $\mathbf{l}$ parallel to $\mathbf{V_b}$ and let

$$\mathbf{X}_j = \mathbf{V_r}_j + s\,\mathbf{l}\,, \tag{4.1.2.4}$$

where s is a constant to be determined. Substituting in (4.1.2.1) we obtain

$$s^2 \mathbf{l}^T \mathbf{A}\mathbf{l} + 2s\, \mathbf{V_r}^T \mathbf{A}\mathbf{l} + \mathbf{V_r}^T \mathbf{A} \mathbf{V_r} - d = 0\,; \tag{4.1.2.5}$$

solving for s we get

$$s = \frac{-\mathbf{V_r}^T \mathbf{A}\mathbf{l} + \sqrt{(\mathbf{V_r}^T \mathbf{A}\mathbf{l})^2 - (\mathbf{l}^T \mathbf{A}\mathbf{l})(\mathbf{V_r}^T \mathbf{A}\mathbf{V_r} - d)}}{\mathbf{l}^T \mathbf{A}\mathbf{l}}\,. \tag{4.1.2.6}$$

The elliptic cone which is tangent to the ellipsoid and which has its apex on the viewpoint can be obtained from the matrix $\mathbf{A}$ and from the vector $\mathbf{V_u}$ which extends from the center of the ellipsoid to the viewpoint. This is performed in the following steps:

1. The ellipsoid is transformed with a rotation matrix to a new Cartesian frame of reference which has the z axis along the view vector $\mathbf{V_u}$.
2. The tangent cone can now be described as

$$\mathbf{Y}^T \mathbf{C} \mathbf{Y} = 0\,, \tag{4.1.2.7}$$

where $\mathbf{Y}$ is a vector originating from the vertex (viewpoint) of the cone and

$$\mathbf{C} = \begin{pmatrix} a_{11} + \dfrac{a_{13}a_{31}}{K-a_{33}} & a_{12} + \dfrac{a_{13}a_{32}}{K-a_{33}} & \dfrac{Ka_{13}}{K-a_{33}} \\[2ex] a_{21} + \dfrac{a_{23}a_{31}}{K-a_{33}} & a_{22} + \dfrac{a_{23}a_{32}}{K-a_{33}} & \dfrac{Ka_{23}}{K-a_{33}} \\[2ex] \dfrac{Ka_{31}}{K-a_{33}} & \dfrac{Ka_{32}}{K-a_{33}} & \dfrac{Ka_{33}}{K-a_{33}} \end{pmatrix}, \quad K = d/(\mathbf{V_u}^T \mathbf{V_u}). \tag{4.1.2.8}$$

3. The frame of reference is rotated back to its original orientation with a rotation matrix which is the inverse of the one used in step 1. Note that the origin is now on the viewpoint rather than the ellipsoid center.

To find the length, s, of a vector $s\,\mathbf{l}$ extending from any point p inside the cone to the surface of the cone we let

$$\mathbf{Y} = \mathbf{V_p} + s\,\mathbf{l} \tag{4.1.2.9}$$

and obtain from (4.1.2.7)

$$(\mathbf{V_p} + s\,\mathbf{l})^T \mathbf{C} (\mathbf{V_p} + s\,\mathbf{l}) = 0\,;$$

then solving for s we obtain

$$s = \frac{-V_p^T C l \pm \sqrt{(V_p^T C l)^2 - (l^T C l)(V_p^T C V_p)}}{l^T C l} \tag{4.1.2.10}$$

The vector V_p from the vertex to p is formed by

$$V_p = -V_0 + V_r ,$$

where V_r is any member of a radial set such as that described for the regular ellipsoid intersection.

4.2 OR TEP Subprograms

The subprograms can be grouped into four functional categories. They can be called Mainstream, Subsidiaries, Arithmetic, and Plotting. The first three categories are coded in a FORTRAN dialect which will compile with either IBM-7090 FORTRAN II or CDC-1604A FORTRAN 63. The plotting routines are generally different for each machine configuration and are usually written in a machine-oriented symbolic language. In general, the standard library plotting routines available at most computing centers can be used with very minor modification.

4.2.1 Mainstream Subprograms. – The first three (PRIME, PRELIM, and MAIN) are the general controlling routines, and the remainder are oriented toward particular OR TEP instructions.

4.2.1.1 PRIME. – This routine "primes the program" by initializing all the "primer parameters" including the magnetic tape logical number assignments.

4.2.1.2 PRELIM. – All calculations concerned with processing (e.g., principal axis transformations) and storing the input crystallographic parameters are performed by PRELIM.

4.2.1.3 MAIN. – MAIN is the controlling routine which decodes the OR TEP instructions. It either executes the command directly or calls the appropriate subroutine which can execute the instruction.

4.2.1.4 F200. – This is the plotter "mermaid routine" which is controlled through the 200 series instructions. It satisfies the whims and fancies of any particular plotting system control package.

4.2.1.5 F400. – This is the subroutine that executes the 401 and 411 instructions.

4.2.1.6 F500. – This is the subroutine that executes all 500 series instructions.

4.2.1.7 F600. – This is the subroutine that executes all 600 series instructions.

4.2.1.8 F700. – This is the ellipsoid plotting routine, which executes all 700 series instructions.

4.2.1.9 F800. – This is the subroutine that executes all 800 series instructions. Bonds to be drawn are found by F800, then drawn by subroutine BOND.

4.2.1.10 F900. – This is the subroutine that executes all 900 series instructions.

4.2.1.11 F1000. – This is a dummy subroutine which is called by the presently nonexistent 1000 series instructions. This series can be coded by the user for any special purpose which may develop.

4.2.1.12 SPARE(NJ). – Further expansion of the instruction list may be done through this dummy subroutine, which is called by any $NJ \geq 12$. $NJ = \text{instruction}/100$.

4.2.2 Subsidiary Subprograms. – 4.2.2.1 ATOM(ADC,X), DIMENSION X(3). – This will find the triclinic coordinates X for the atom described by the atom designator code ADC.

4.2.2.2 BOND (ADC1, ADC2, NB). – BOND is the bond plotting routine to draw a bond, described by Format No. 2 trailer card number NB, between atoms ADC1 and ADC2.

4.2.2.3 DRAW (W,DX,DY,NPEN), DIMENSION W(3). – DRAW interconnects ORTEP and the plot package. It also prevents the pen from crossing the boundaries. If the indicator ITILT in common is zero, the array W contains x and y in plotter coordinates. While perspective lettering is being plotted, ITILT ≠ 0, and W contains x, y, z in Cartesian coordinates, which will be rotated and projected by DRAW to form plotter x,y coordinates. *DX* and *DY* are added to the plotter x and y, respectively, before the plot package is called. NPEN = 2 for pen down and 3 for pen up.

4.2.2.4 ERPNT (ADC,INST). – This is the printout routine called when a Fault is found. The arguments identify the atom designator code and the instruction involved in the Fault. The fault indicator, NG, is in common.

4.2.2.5 PAXES (ADC,ITYPE). – The covariance (dispersion) matrix for the thermal ellipsoid or its inverse matrix, which is the matrix of coefficients in the quadratic form describing the ellipsoid, is stored in common at *Q* for the atom ADC.

ITYPE > 0 for covariance matrix
ITYPE < 0 for ellipsoid quadratic form matrix
|ITYPE| = 1 based on triclinic system
|ITYPE| = 2 based on working Cartesian system
|ITYPE| = 3 based on reference Cartesian system

4.2.2.6 PLTXY (X,Y), DIMENSION X(3),Y(2). – This calculates the plotter coordinates *Y* from the unscaled Cartesian coordinates *X*. The distance to the closest boundary of the plot is placed in common at location EDGE.

4.2.2.7 PROJ (D,DP,X,XO,VIEW,I1,I2,I3), DIMENSION D(3,129),DP(2,129),X(3),XO(3). – This routine is used to obtain an array, DP, of plotter coordinates from a scaled array, D, of points described in Cartesian coordinates. X, XO, and VIEW are parameters involved in the projection, and I1, I2, I3 are DO loop parameters for indexing through the array.

4.2.2.8 RADIAL(ND). – Given two conjugate radius vectors of an ellipse in the array DA in common, RADIAL generates a "radial" array (D in common) of points lying on the ellipse. From 8 to 128 points are generated depending on the value of ND ($1 \leq ND \leq 5$).

4.2.2.9 SEARCH. – Instructions 101, 102, 402, and 403 utilize this routine to conduct an exhaustive (but educated) search to find all points within a sphere or rectangular box. Interatomic distances and angles are also calculated for the 100 series.

4.2.2.10 STORE. – This routine stores atoms in (or removes atoms from) the ATOMS array. Coordinates in whichever system is in use and the atom designator code are communicated to STORE via array V1 of common.

4.2.2.11 XYZ(ADC,X,ITYPE), DIMENSION X(3). – Coordinates for atom ADC are returned in *X*.

ITYPE = 0: triclinic coordinates

ITYPE = 1 or 2: working Cartesian system coordinates

ITYPE = 3: reference Cartesian system coordinates

4.2.2.12 **LAP500.** – This routine sorts the ATOMS list, then calculates the projected outline ellipses for all atoms in the ATOMS list. The ellipses are stored in the CONIC array along with the minima and maxima in x and y for a rectangle enclosing each ellipse.

4.2.2.13 **LAP700.** – This routine finds the atoms which overlap a given atom to be drawn. The routine first checks the bounding rectangles for intersections, then forms the cubic discriminant from the quadratic descriptions of the two projection ellipses. The discriminant provides a specification for complete overlap, partial overlap or no overlap. A list of up to 20 interfering ellipses is compiled.

4.2.2.14 **LAP800.** – This routine is used in the "Projected Outline Storage Step" to store the projected quadrangles for the bonds specified by the trailer cards of the 511, 821, and 822 instructions. The routine also is used in the "Area–Overlap Search Step" to find the projected bond quadrangles which overlap a given bond to be drawn. A list containing up to thirty interfering quadrangles is compiled.

4.2.2.15 **LAPAB.** – This routine finds the bonds that overlap an atom to be drawn and the atoms that overlap a bond to be drawn. It is used in the "Area–Overlap Search Step."

4.2.2.15 **LAPDRW.** – This routine checks each line segment to be drawn for intersection with the interfering ellipses and quadrangles and compiles a list of intersections. The intersection list is sorted according to distance along the line segment, and the intersection pattern is analyzed to determine which subsegments are visible and which are hidden. The line subsegments are passed to the SCRIBE routine.

4.2.2.17 **SCRIBE.** – This routine filters out the hidden line segments and passes the visible line segments to the DRAW routine.

4.2.3 Arithmetic Subprograms. – 4.2.3.1 **Function ARCCOS (X).** – This routine computes θ, the arc cosine of X in degrees; $0 \leqq \theta \leqq 180°$.

4.2.3.2 **AXEQB (A,X,B,N), DIMENSION A(3,3),X(3,3),B(3,3).** – This routine solves the matrix equation **A X = B** for **X**. The matrices **B** and **X** are (3,N) and **A** is always (3,3). To invert **A**, make **B** an identity matrix.

4.2.3.3 **AXES (X, Y, A, ITYPE), DIMENSION X(3),Y(3),A(3,3).** – This routine provides three orthogonal column vectors in **A**, each 1 A long, from the two vectors **X** and **Y**.

ITYPE > 0: Cartesian system

ITYPE $\leqq 0$: triclinic system

$|\mathrm{ITYPE}| = 1$: $A_1 = X$; $A_2 = (X \times Y)$; $A_3 = X \times (X \times Y)$

$|\mathrm{ITYPE}| = 2$: $A_1 = X$; $A_2 = (X \times Y) \times X$; $A_3 = X \times Y$

ITYPE $= 0$: same as type 2 except $X = a$ crystal axis, $Y = b$ crystal axis.

4.2.3.4 **DIFV (X,Y,Z), DIMENSION X(3),Y(3),Z(3).** – This routine performs the vector subtraction $X - Y = Z$. Z may have the same location as X or Y.

4.2.3.5 **EIGEN (A,X,B), DIMENSION A(3,3),X(3),B(3,3).** – EIGEN determines the three eigenvalues **X** and the three column eigenvectors **B** of the matrix **A**. Indeterminate eigenvectors are replaced by zeros and the Fault indicator NG set to a negative value (eigenvectors are assigned for the indeterminate cases by PRELIM).

4.2.3.6 **MM (A,B,C), DIMENSION A(3,3),B(3,3),C(3,3).** — MM performs the matrix multiplication A B = C. The location of C must be different from A and B.

4.2.3.7 **MV (A,X,Y), DIMENSION A(3,3),X(3),Y(3).** — MV performs the matrix-vector multiplication A X = Y. The location of Y must be different from A and X.

4.2.3.8 **NORM (X,Y,Z,ITYPE), DIMENSION X(3),Y(3),Z(3).** — NORM stores at Z a vector (not necessarily a unit vector) perpendicular to both X and Y. The sense of Z is that of the vector product X × Y.

ITYPE > 0: Cartesian system

ITYPE ≤ 0: triclinic system

4.2.3.9 **TMM (A,B,C), DIMENSION A(3,3),B(3,3),C(3,3).** — TMM performs the matrix multiplication $(A^T B)^T = C$. The location of C must be different from A and B.

4.2.3.10 **UNIT (X,Y,ITYPE), DIMENSION X(3),Y(3).** — The vector Y is made 1 A long and parallel to X. The vectors X and Y may have the same location.

ITYPE > 0: Cartesian system

ITYPE < 0: triclinic system

4.2.3.11 **VM (X,A,Y), DIMENSION X(3),A(3,3),Y(3).** — VM performs the vector-matrix multiplication $X^T A = Y^T$. The location of Y must be different from X and A.

4.2.3.12 **FUNCTION VMV (X,A,Y), DIMENSION X(3),A(3,3),Y(3).** — VMV performs the vector-matrix-vector multiplication $X^T A Y$ = scalar.

4.2.3.13 **FUNCTION VV (X,Y), DIMENSION X(3),Y(3).** — VV performs the vector-vector multiplication $X^T Y$ = scalar.

4.2.4 **Plotting Subprograms for the CalComp Plotter.** — The plotting subroutines are taken from the Library routines currently in use at Oak Ridge National Laboratory with the CDC 1604A and the IBM 7090 computers. A CalComp model 580 Magnetic Tape Plotting System is used. The three major routines required are derived from the CalComp subroutines PLOTS, SYMBOL, and NUMBER. The OR TEP modifications are called PLOTS, SIMBOL, and NUMBUR.

4.2.4.1 **Subroutine PLOTS.** — This is an unmodified CalComp Library routine with two entry points.

a) ENTRY — PLOTS (A, LENGTH, LTNO)

This is the initialization entry for the plotter package and should be used only once in the program. This call must be made prior to usage of any other subroutines in the package.

A is an array which may be used by the plotting package for storing data to be written on the plot tape.

LENGTH is the number of locations in A available to the plotter package.

LTNO is an integer which tells the plotter package the logical tape number of the plotter tape.

In subroutine F200 we have

DIMENSION PLA(1500)

and card F2000180 contains

"210 CALL PLOTS (PLA,1500, LTNO)"

for the CDC 1604-A or

"210 CALL PLOTS (PLA(1500),1500,LTNO)"

for the IBM 7090. The reverse storage of common in the IBM 7090 is the reason for the difference. LTNO is in common and was set to 23 by subroutine PRIME.

An ORTEP 201 instruction directs the execution of this initialization.

b) ENTRY – PLOT (X,Y,IPEN)

This is the basic entry to convey data to the subroutine for plotting. To facilitate the substitution of other plotting routines, ORTEP contains only one instruction (card DRAW0330 in subroutine DRAW) which calls this entry point. All the plotting information passes through DRAW before going to the actual plotting routine PLOT.

X is the abscissa expressed in inches.

Y is the ordinate expressed in inches.

IPEN = 3, the pen will be lifted prior to execution of the movement to the given (X,Y) position.

IPEN = 2, the pen will be lowered to the paper and a straight line will be drawn from the current (X,Y) to the given (X,Y) position.

IPEN = −3, the subroutine will interpret this as being the end of the current plot; and, following movement to the new (X,Y) position, it will set X = 0.0, so that a new origin is established for the following plot (an ORTEP 202 instruction executes this termination procedure).

This subroutine keeps track of current X and Y positions, and whether or not the pen is in contact with the paper. It stores data in the array A provided by the programmer and writes out a record on the specified tape each time the storage area is filled or an end-of-plot call is made. It also generates sequential plot addresses for each plot on the magnetic tape, so that physical plotting of the plots can be done in any order, regardless of the order in which they were placed on tape.

4.2.4.2 Subroutine SIMBOL. – SIMBOL differs from the standard routine SYMBOL in two respects:

1. The input positional parameters specified in the input argument should be an array containing *X*, *Y*, and *Z* in adjacent memory locations. Three-dimensional parameters are required to produce perspective labels. The *Z* parameter is not used by SIMBOL but is transferred to another array that is referenced when SIMBOL calls DRAW.

2. The standard routine SYMBOL calls PLOT directly while SIMBOL calls DRAW which in turn calls PLOT. When perspective labels are used, DRAW will perform a three-dimensional rotation and a projection of the grid points on which the letters are formed, to obtain true perspective. The calling sequence for DRAW is described in 4.2.2.3.

There are two uses of subroutine SIMBOL. The first use is for producing labels, and the second is for plotting one of 15 special centered symbols.

1. ENTRY – SIMBOL (X(1),X(2),H,BCD,THETA,N), DIMENSION X(3) (note $N \geq 0$)

   X(1),X(2) are the X and Y coordinates of the lower left-hand edge of the first character to be drawn.

   X(3) is the Z coordinate. It is used only with perspective labeling.

   H is the height in inches of the character to be drawn. The width of the character is equal to $^4/_7$ the height and the character spacing is $^6/_7$ the height.

   BCD specifies the address of an array containing the BCD characters to be plotted.

   THETA is the angle in degrees by which the base line of the characters is to be rotated counterclockwise from the positive X axis.

   N is an integer which specifies the number of characters in the array BCD that are to be drawn.

2. ENTRY – SIMBOL (X(1),X(2),H,NUM,THETA,L), DIMENSION X(3) (note $L < 0$)

   X(1),X(2) are the X and Y coordinates of the center of the symbol.

   H is the height of the symbol to be plotted.

   NUM is an integer such that $0 \leq \mathrm{NUM} \leq 14$ which determines which symbol is to be plotted. A list of the integers and the symbols generated is shown in Fig. 4.2.

   THETA is the angle of rotation as described previously.

   $L = -1$: the centered symbol will be plotted without a line being drawn from the previous (X,Y) position.

   $L < -1$: a straight line will be drawn from the previous (X,Y) position to the given (X,Y) position.

4.2.4.3 Subroutine NUMBUR. – This is a subroutine to convert a machine format number to its BCD equivalent and plot it according to a specified format.

NUMBUR is different from the usual subroutine NUMBER in that it calls SIMBOL rather than SYMBOL.

ENTRY – NUMBUR(X(1),X(2),H,A,THETA,N)

X(1),X(2),H and THETA are described in Sect. 1 of the SIMBOL routine

A is the address of the floating or fixed point number which is to be plotted.

N is the number of digits to the right of the decimal point. A(–1) value will suppress the decimal point.

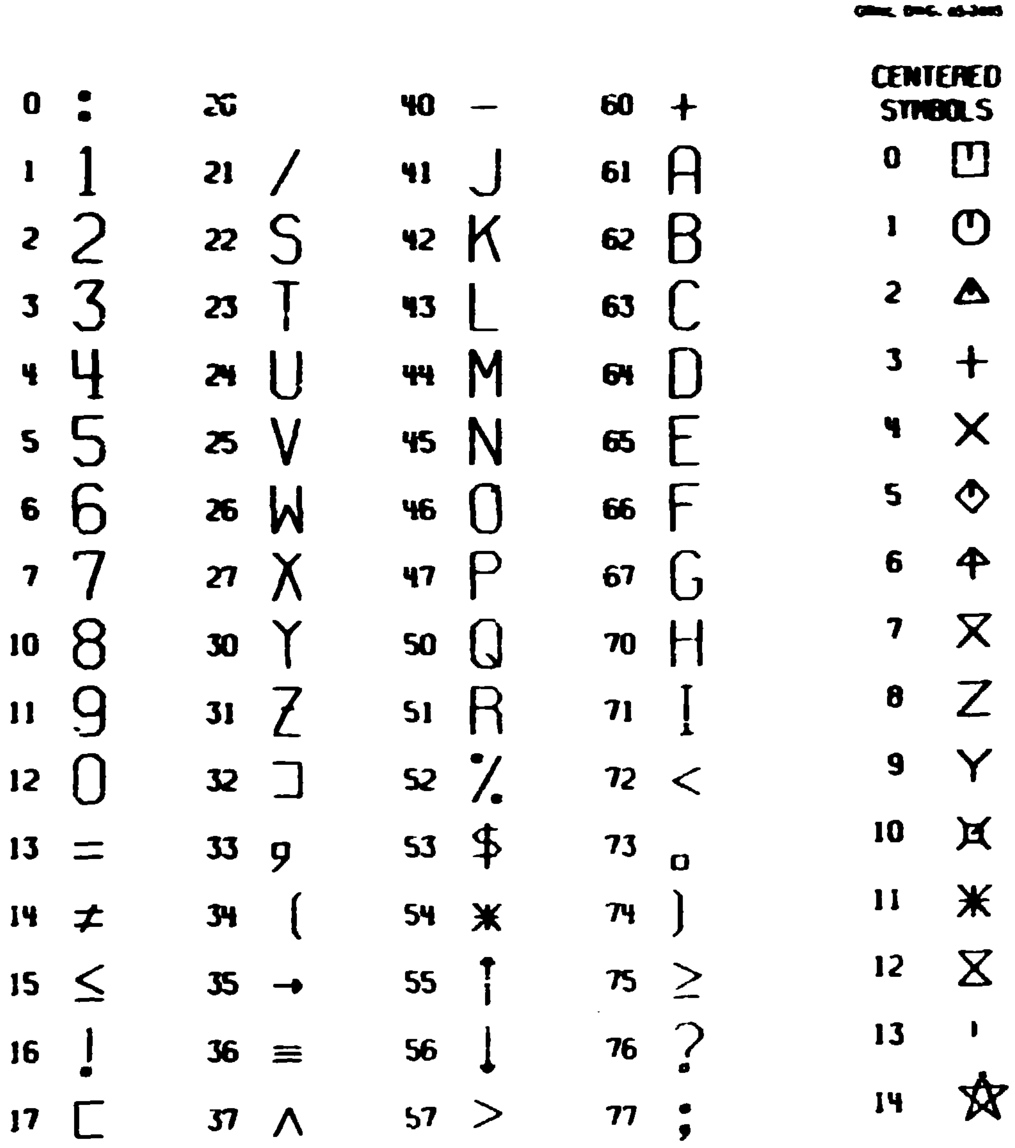

Fig. 4.2. Characters Available in 1604-A Symbol Routine.

4.3 Adapting OR TEP to Other Equipment Configurations

Card images[2] for OR TEP will be provided to crystallographers and others who request that the program be sent to them.

FORTRAN decks are available in IBM 360 FORTRAN IV and IBM 7090 FORTRAN IV. The FORTRAN subprograms are arranged alphabetically within the FORTRAN source decks. An exception is MAIN, which is first in each deck.

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[2] The size of the card deck (3000–6000 cards) is such that it is generally more economical to send the program on magnetic tape. If convenient, the user should send a blank magnetic tape to the author. Card images will be written on that tape in an agreed upon format and the tape returned to the sender.

The machine language subroutines SIMBOL and NUMBUR are modifications of the CalComp subroutines SYMBOL and NUMBER. Subroutine PLOT is an unmodified CalComp subroutine also written in machine language. These three subroutines are copyrighted by California Computer Products, Inc. Subroutines SIMBOL and NUMBUR for IBM 360, IBM 7090, and CDC 1604-A can be distributed from ORNL. Subroutine PLOT which is different for each plotter may be obtained from California Computer Products, Inc., 305 Muller Avenue, Anaheim, California (Attention: Programming Dept.).

Cards for the example figure, cubane, will be included with the deck.

4.3.1 OR TEP Source Deck Differences for the IBM 360 and the IBM 7090. – The listing of the FORTRAN IV source deck for the IBM 360 is given in Sect. 7. The length of the single-precision floating-point word in the IBM 360 is such that the maximum number of atoms in the input list cannot be greater than 166 because of the way the atom designators are stored. This must be taken into account if the dimension statements of the program are changed.

The following changes are made to modify the program for IBM 7090 FORTRAN IV:

1. Remove the "REAL*8 CHEM" card from the subprograms which use common.
2. Add the correct IBSYS monitor control cards including "$POOL" and "$GROUP" cards to conserve memory space.

The following changes are made to modify the program for IBM 7090 FORTRAN II:

1. Remove the "REAL*8 CHEM" cards from the subprograms which use common.
2. Add "*LIST8" and "*LABEL" cards before each subprogram.
3. Replace card F2000180 with "210 CALL PLOTS (PLA(1500), 1500,LTNO)."
4. Change input-output statements and library function names to correspond with FORTRAN II convention.

4.3.2 External Device Logical Number Assignments. – Logical device number assignments are made in subroutine PRIME. Four cards are involved in this initialization:

Magnetic Tape Function	Symbolic Name		Primer Constant	Location in PRIME
a) Monitor Input	IN	=	5	PRIM0220
b) Monitor Output	NOUT	=	6	PRIM0280
c) Scratch	NSR	=	8	PRIM0290
d) Plotting	LTNO	=	23	(PRIM0250)*

4.3.3 Plotter Systems Other than the CalComp 500. – In general, only subroutine PLOTS (with entries PLOTS and PLOT) needs to be replaced when a different plotting system is used. This routine is called from only two locations, one in F200 and the other in DRAW. F200 will probably have to be rewritten, and

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*In the present revision, LTNO also serves as a plotting device indicator and is initialized to zero at MAIN0145. For the mechanical plotter (CRT), LTNO is set to 15 (−99) at F2000210 (F200250) by a 201 (203) instruction.

the 200 series instructions may have to be redefined and expanded to accommodate the rules of the new system.

Location DRAW9330 in subroutine DRAW should also be modified to call the new line-drawing routine with the correct argument.

4.3.4 Computing Systems Other Than the IBM 360, IBM 7090, and CDC 1604-A. – Basically, the OR TEP system is designed to be used as ≥ 32 K memory. Consequently, OR TEP would have to be changed considerably to operate in a much smaller memory.

The FORTRAN coding of OR TEP has proven to be fairly machine independent, but as compilers become more sophisticated new problems continually appear. For example, some compilers rearrange the sequence of operations to obtain more efficient execution and sometimes they "outsmart" themselves in the process. Certain of the 6000 series CDC compilers occasionally take an instruction such as II = ATOMS(I,J)/100000. and make it into TEMP = 1./100000., II = ATOMS(I,J)*TEMP. The effect is disastrous because the numerical rounding and truncation produce an incorrect integer II.

If it becomes necessary to replace the machine language subroutines SYMBOL and NUMBUR with completely different routines, the statements calling these routines will also need to be modified.

SYMBOL is called from BOND0460, BOND0480, F7060850, F9601310, F9001340, and F9001470.

NUMBUR is called from BOND 2510 and F9001440.

4.3.5 Space Requirements with Overlap Feature. – The overlap feature requires an additional block of approximately 15 K words of computer memory and will cause ORTEP to exceed the memory of a 32 K computer. For computers with a working storage under 45 K-60 K words, the overlap feature may be deleted by removing subroutines LAP500, LAP700, LAP800, LAPDRW, LAPAB, and LAPCON and substituting dummy subroutines for the first four of these six subroutines.

4.4 Addition of New OR TEP Instructions

Occasions will arise when additional special purpose instructions would be useful. For example, perhaps a cell outline routine would be desirable. (Originally, the 1000 series of instructions were planned for drawing a parallelepiped defined by four general vectors. However, this feature later seemed somewhat redundant and was omitted, since crystal cell outlines can be produced with judicious usage of small dummy atoms and the 800 series instructions.)

The subroutines F1000 and SPARE are intended to be used for additional instructions. All 1000 series instructions call subroutine F1000, which is currently just a dummy routine. Instructions ≥ 1200 call another dummy routine, subroutine SPARE(NJ), where NJ – instruction number 100.

All Arithmetic subprograms (see 4.2.3) and many of the subsidiary subprograms (see 4.2.2) are available for coding these Mainstream subprograms (see 4.2.1).

4.5 Glossary of Symbols in ORTEP Common, with Array Dimensions

	A(9)	Direct crystal cell parameters, a, b, c, cos α, cos β, cos γ, [illegible]
	AA(3,3)	Metric tensor g where $g_{ij} = \mathbf{a}_i \cdot \mathbf{a}_j$.
	AAREV(3,3)	Postfactor transformation matrix to convert coordinates from triclinic to the reference Cartesian system. AAREV = AA REFV.
	AAWRK(3,3)	Postfactor transformation matrix to convert coordinates from triclinic to the working Cartesian system. AAWRK = AA WRKV.
	AID(3,3)	Identity matrix.
	AIN(140)	Array containing the input parameters of the current ORTEP instruction.
	ATOMS(4,500)	Column 1 contains atom designator codes for the atoms which are to be included in the scaling, plotting, bond searching, etc. The other three columns are used for temporary storage of coordinates in any of several coordinate systems.
	BB(3,3)	Reciprocal metric tensor. BB = AA^{-1}.
P	BRDR	Border width in inches extending inward from plot boundary.
	CD(8,10)	Part of vector search code array. Used in conjunction with KD array.
	CHEM(100)	Chemical symbols for the input atoms.
P	CONT(5)	Constants used in subroutine RADIAL.
	D(3,130)	Array in which three-dimensional points on an ellipse are stored by RADIAL.
	DA(3,3)	Transmits conjugate vectors to RADIAL. Also used for temporary storage.
	DP(2,130)	Array in which two-dimensional points for ellipse are stored after projection.
P	DISP	Displacement parameter for retracing.
	EDGE	Distance in inches from a projected point to the closest boundary. Set in PLTXY.
	EV(3,100)	Root-mean-square displacements for each principal axis of each input atom.
P	FORE	Cosine of critical angle between bond and Cartesian z axis vectors for perspective bond distance labels. At smaller angles the labels, produced from subroutine BOND, are drawn without perspective to prevent excessive foreshortening.
	FS(3,3,48)	Rotation matrices for input symmetry operations based on triclinic system. Used with TS array.
P	IN	Logical number for monitor input magnetic tape.
P	ITILT	Indicator used to signal subroutine DRAW, whether or not to do perspective labeling ("Tilted Titles").
	KD(5,10)	Part of vector search code array. Used in conjunction with CD.
P	LATM	Number of entries in ATOMS array.
P	LTNO	Logical tape number for magnetic plotting tape.
	NATOM	Number of input atoms.
P	NCD	Number of Format No. 2 trailer cards for an instruction (vector search codes).

Note: (P) indicates "prime parameters," which are initialized in subroutine PRIME.

P	NG	FAULT INDICATOR (see 3.4).
	NJ	Instruction number/100.
	NJ2	Last two decimal digits of the instruction number (instruction = NJ*100 + NJ2).
P	NOUT	Logical number for monitor output magnetic tape.
P	NSR	Logical number for scratch magnetic tape.
	NSYM	Number of input symmetry operations.
P	ORGN(3)	Triclinic coordinates for the atom which is the origin of the drawing (i.e., on the optic axis for the projection).
	P(3,100)	Triclinic positional coordinates for the input atoms.
	PA(3,3,100)	Matrices for each input atom made up of three orthogonal column eigenvectors each 1 Å long, based on the triclinic system (principal axis vectors).
	PAC(3,5)	A 3 × 3 matrix produced by subroutine PAXES and made up of three orthonormal principal axis column vectors, based on either the working or reference Cartesian system. Columns 4 and 5 are used in subroutine F700 to duplicate columns 1 and 2 for ease in indexing.
	PAT(3,3)	A matrix produced by subroutine PAXES and composed of three principal axis column vectors each 1 Å long, based on the triclinic system.
	Q(3,3)	A matrix produced by subroutine PAXES. Contains either the dispersion matrix or its inverse, based on either the working or reference Cartesian systems.
	REFV(3,3)	A matrix made up of three orthogonal column vectors, each 1 Å long, based on the triclinic system. This is the base vector triplet for the reference Cartesian coordinate system. The transpose is the postfactor transformation matrix for converting coordinates from the reference orthogonal system to the triclinic system. $\mathbf{REFV}^T = \mathbf{AAREV}^{-1}$.
P	RES(4)	Regulates the resolution of the plotting of a given ellipse as a function of the longest principal axis x in the given ellipsoid of the scaled model. $x \le$ Res(1) 128-point ellipse Res(1) $< x \le$ Res(2) 64-point ellipse Res(2) $< x \le$ Res(3) 32-point ellipse Res(3) $< x$ 16-point ellipse Res(4) is not used.
	RMS(5)	The rms displacements along the principal axes in arrays PAC and PAT.
P	SCAL1	The scale of the model in inches per angstrom before projection.
P	SCAL2	The scale factor ratio which sets the ellipsoid scale relative to SCAL1. If SCAL2 = 1.54, then the instantaneous position of the atomic center will be within the ellipsoid 50% of the time (50% probability ellipsoid).
P	SCL	SCL = SCAL1 times SCAL2.
P	SYMB(3,3)	A rotation matrix based on the angle THETA which is set by instruction 302.
P	TAPER	The exaggerated bond taper parameter. The top and bottom ends of a bond have radii: RADIUS - 1. + TAPER *T6 where T6 = cosine of angle between bond and z axis of Cartesian system.

Note: (P) indicates "prime parameters," which are initialized in subroutine PRIME.

P	THETA	Angle in degrees between plotter x axis and lettering base-line vector.
	TITLE(12)	Alphanumeric job title storage.
	TITLE2(12)	Alphanumeric information storage for Format No. 3 trailer card.
	TS(3,48)	Translation vector for each input symmetry operation. Used with FS array.
P	VIEW	Viewing distance in inches.
	VT(3,4)	Perspective title rotation matrix and translation vector. Also used for temporary storage.
	V1(4)	Array to transfer data to subroutine STORE. Also used for temporary storage.
	V2(3) , ... , V6(3)	Temporary storage.
	WRKV(3,3)	Same definition as for REFV except that this one is for working Cartesian system. $\mathbf{WRKV}^T = \mathbf{AAWRK}^{-1}$.
P	XLNG(3)	Elements (1) and (2) are x and y plot dimensions. Element (3) is not used.
P	XO(3)	Elements (1) and (2) denote the position in plotter coordinates (in inches) where ORGN is placed. Element (3) is used to transfer Z coordinates to subroutine DRAW when perspective lettering is used.
	XT(3)	Triclinic coordinates for an atom position are placed here by subroutine XYZ.

Note: (P) indicates "prime parameters," which are initialized in subroutine PRIME.

5. MATHEMATICS OF THERMAL-MOTION PROBABILITY ELLIPSOIDS

It is convenient to develop the physical significance of the anisotropic temperature factor with the notation and terminology of probability theory rather than with the more familiar Fourier transform theory. The results are, of course, identical regardless of the terminology used. The reason for this choice is that the literature of mathematical statistics and probability theory is somewhat neater and easier to follow. The texts by Wilks,[1] Cramer,[2] Miller,[3] Hamilton,[4] and Lukacs and Lana[5] and the handbooks by Burington and May[6] and Owen[7] are found to be particularly useful.

5.1 Probability Density Function (pdf) of a Trivariate Normal Distribution

Given three chance variables X_1, X_2, X_3 and S which is a region in X_1, X_2, X_3 space. The probability $P(S)$ that the point (X_1, X_2, X_3) falls in the region S is given by

$$P(S) = \iiint_S \phi(X_1, X_2, X_3)\, dX_1\, dX_2\, dX_3 \; . \tag{5.1.1}$$

If the integration is carried over all space, then

$$\iiint_{-\infty}^{\infty} \phi(X_1, X_2, X_3)\, dX_1\, dX_2\, dX_3 = 1 \; . \tag{5.1.2}$$

The function $\phi(X_1, X_2, X_3)$ is called the probability density function (pdf) for the joint distribution of X_1, X_2, X_3. Using vector notation, we can designate the pdf as $\phi(\mathbf{X})$.

When the distribution is the type said to be normal or Gaussian, the pdf is

$$\phi(\mathbf{X}) = \frac{[\det(\mathbf{M}^{-1})]^{1/2}}{(2\pi)^{3/2}} \exp[-\tfrac{1}{2}(\mathbf{X} - \hat{\mathbf{X}})^T \mathbf{M}^{-1}(\mathbf{X} - \hat{\mathbf{X}})] \; . \tag{5.1.3}$$

The matrix $\mathbf{M}^{-1}$ is the inverse of the symmetrical dispersion (variance-covariance) matrix $\mathbf{M}$, where

$$\mathbf{M} = \begin{pmatrix} \sigma_1^2 & \sigma_1\sigma_2\rho_{12} & \sigma_1\sigma_3\rho_{13} \\ \sigma_1\sigma_2\rho_{12} & \sigma_2^2 & \sigma_2\sigma_3\rho_{23} \\ \sigma_1\sigma_3\rho_{13} & \sigma_2\sigma_3\rho_{23} & \sigma_3^2 \end{pmatrix} \; .$$

The symbols σ_i^2 represent the second moments or variances about the mean position $\hat{\mathbf{X}}$. The symbols $\sigma_i\sigma_j\rho_{ij}$ are the corresponding covariances and ρ_{ij} are the correlation coefficients.

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[1] S. S. Wilks, *Mathematical Statistics*, Wiley, New York, 1962.

[2] H. Cramer, *Random Variables and Probability Distributions*, Cambridge University Press, London, 1962.

[3] K. S. Miller, *Multidimensional Gaussian Distributions*, Wiley, New York, 1964.

[4] W. C. Hamilton, *Statistics in Physical Science*, Ronald, New York, 1964.

[5] E. Lukacs and R. G. Lana, *Applications of Characteristic Functions*, Hafner Publishing Co., New York, 1964.

[6] R. S. Burington and D. C. May, *Handbook of Probability and Statistics with Tables*, Handbook Publishers, Sandusky, Ohio, 1953.

[7] D. B. Owen, *Handbook of Statistical Tables*, Addison-Wesley, Reading, Mass., 1962.

5.2 Equiprobability Ellipsoids

For a proper normal distribution the quadratic form $(\mathbf{X}-\hat{\mathbf{X}})^T\mathbf{M}^{-1}(\mathbf{X}-\hat{\mathbf{X}})$ is positive definite, and a principal axis transformation is possible which will make the cross correlation coefficients $\rho_{ij} = 0$ $(i \neq j)$. This transformation is discussed in 5.4. The result of the transformation is the pdf

$$\phi(y_1, y_2, y_3) = \frac{1}{(2\pi)^{3/2}\sigma_{y_1}\sigma_{y_2}\sigma_{y_3}} e^{-Q/2} . \tag{5.2.1}$$

where

$$Q = \frac{(y_1-\hat{y}_1)^2}{\sigma_{y_1}^2} + \frac{(y_2-\hat{y}_2)^2}{\sigma_{y_2}^2} + \frac{(y_3-\hat{y}_3)^2}{\sigma_{y_3}^2} . \tag{5.2.2}$$

The y_i are coordinates based on the Cartesian principal axis system and $\sigma_{y_i}^2$ are the variances along the principal axes, $i = 1, 2, 3$.

The normal probability density function is constant for points on the ellipsoid $Q = C^2$ where C is a constant. The probability that a random point (y_1, y_2, y_3) in the distribution will fall inside the ellipsoid is

$$P(C) = (2/\pi)^{1/2} \int_0^C r^2 e^{-r^2/2}\, dr . \tag{5.2.3}$$

This result is derived from (5.1.1), (5.2.1), and (5.2.2) by transforming to spherical coordinates.

When $C = 1.5382$, $P = 0.5$ and the corresponding ellipsoid is called the 50% probability ellipsoid. A table of P vs C values is found on page 203 of Owen's *Handbook of Statistical Tables*.[7] For convenience, that table is reproduced here as Table 5.1.

5.3 Characteristic Function (c.f.) of a Trivariate Normal Distribution

The characteristic function $\Phi(\mathbf{T})$ corresponding to a trivariate distribution $\phi(\mathbf{X})$ is the expected value of $e^{i\mathbf{T}^T\mathbf{X}}$, namely,

$$\Phi(\mathbf{T}) = \int_{-\infty}^{\infty} \phi(\mathbf{X})\, e^{i\mathbf{T}^T\mathbf{X}}\, d\mathbf{X} . \tag{5.3.1}$$

For the trivariate normal pdf (5.1.3) the corresponding characteristic function is

$$\Phi(\mathbf{T}) = \exp\left[i\,\mathbf{T}^T\hat{\mathbf{X}} - \tfrac{1}{2}\mathbf{T}^T\mathbf{M}\mathbf{T} \right] , \tag{5.3.2}$$

where $\mathbf{M}$ is the variance-covariance dispersion matrix described in 5.1 and $\hat{\mathbf{X}}$ is the center of mass of the distribution.

The crystallographic structure factor equation which incorporates general anisotropic temperature factor coefficients is

$$F(\mathbf{h}) = \sum_n f_n(\mathbf{h}) \exp(2\pi i\, \mathbf{h}^T\hat{\mathbf{X}}_n) \exp(-\mathbf{h}^T\mathbf{B}_n\mathbf{h}) , \tag{5.3.3}$$

Table 5.1. Critical values for probability ellipsoids of a trivariate normal distribution[a]

P	C	P	C	P	C
0.01	0.3389	0.41	1.3842	0.81	2.1824
0.02	0.4299	0.42	1.4013	0.82	2.2114
0.03	0.4951	0.43	1.4183	0.83	2.2416
0.04	0.5479	0.44	1.4354	0.84	2.2730
0.05	0.5932	0.45	1.4524	0.85	2.3059
0.06	0.6334	0.46	1.4695	0.86	2.3404
0.07	0.6699	0.47	1.4866	0.87	2.3767
0.08	0.7035	0.48	1.5037	0.88	2.4153
0.09	0.7349	0.49	1.5209	0.89	2.4563
0.10	0.7644	0.50	1.5382	0.90	2.5003
0.11	0.7924	0.51	1.5555	0.91	2.5478
0.12	0.8192	0.52	1.5729	0.92	2.5997
0.13	0.8447	0.53	1.5904	0.93	2.6571
0.14	0.8694	0.54	1.6080	0.94	2.7216
0.15	0.8932	0.55	1.6257	0.95	2.7955
0.16	0.9162	0.56	1.6436	0.96	2.8829
0.17	0.9386	0.57	1.6616	0.97	2.9912
0.18	0.9605	0.58	1.6797	0.98	3.1365
0.19	0.9818	0.59	1.6980	0.99	3.3682
0.20	1.0026	0.60	1.7164	0.991	3.4019
0.21	1.0230	0.61	1.7351	0.992	3.4390
0.22	1.0430	0.62	1.7540	0.993	3.4806
0.23	1.0627	0.63	1.7730	0.994	3.5280
0.24	1.0821	0.64	1.7924	0.995	3.5830
0.25	1.1012	0.65	1.8119	0.996	3.6492
0.26	1.1200	0.66	1.8318	0.997	3.7325
0.27	1.1386	0.67	1.8519	0.998	3.8465
0.28	1.1570	0.68	1.8724	0.999	4.0331
0.29	1.1751	0.69	1.8932	0.9991	4.0607
0.30	1.1932	0.70	1.9144	0.9992	4.0912
0.31	1.2110	0.71	1.9360	0.9993	4.1256
0.32	1.2288	0.72	1.9580	0.9994	4.1648
0.33	1.2464	0.73	1.9804	0.9995	4.2107
0.34	1.2638	0.74	2.0034	0.9996	4.2661
0.35	1.2812	0.75	2.0269	0.9997	4.3365
0.36	1.2985	0.76	2.0510	0.9998	4.4335
0.37	1.3158	0.77	2.0757	0.9999	4.5943
0.38	1.3330	0.78	2.1012	0.99999	5.0894
0.39	1.3501	0.79	2.1274	0.999999	5.5376
0.40	1.3672	0.80	2.1544	0.9999999	5.950[illegible]

[a] Reproduced from Ref. 7 by permission of Addison-Wesley Publishing Company, Inc., Reading, Mass. The original caption was "Critical Values for the Spherical Normal Distribution."

where

$\mathbf{h}$ is a vector giving the Miller indices,

$\mathbf{X}_n$ is a vector giving the fractional unit cell coordinates of the nth atom,

$\mathbf{B}_n$ is the anisotropic temperature factor coefficient matrix, and

$f_n(\mathbf{h})$ is the atom form factor value for atom n.

If a change of variables $\mathbf{T} = 2\pi\mathbf{h}$ is made, then (5.3.3) can be rewritten as

$$F(\mathbf{T}) = \sum_n f_n(T) \exp \left(i \mathbf{T}^T \hat{\mathbf{X}}_n - \tfrac{1}{2} \mathbf{T}^T \frac{\mathbf{B}_n}{2\pi^2} \mathbf{T} \right. . \tag{5.3.4}$$

The scaled anisotropic temperature factor matrix $(1/2\pi^2)\mathbf{B}$ is seen to be identical with the variance-covariance dispersion matrix $\mathbf{M}$ in (5.3.2).

The corresponding crystal space trivariate normal pdf for any particular atom n is

$$\phi(\mathbf{X}) = \frac{[2\pi^2 \det(\mathbf{B}^{-1})]^{1/2}}{(2\pi)^{3/2}} \exp[-\pi^2(\mathbf{X} - \hat{\mathbf{X}})^T \mathbf{B}^{-1}(\mathbf{X} - \hat{\mathbf{X}})] ; \tag{5.3.5}$$

or if $\mathbf{M}^{-1} = 2\pi^2\mathbf{B}^{-1}$ then

$$\phi(\mathbf{X}) = \frac{\det(\mathbf{M}^{-1})}{(2\pi)^{3/2}} \exp[-\tfrac{1}{2}(\mathbf{X} - \hat{\mathbf{X}})^T \mathbf{M}^{-1}(\mathbf{X} - \hat{\mathbf{X}})] . \tag{5.3.6}$$

which is identical to (5.1.3).

5.4 Principal Axis Transformation

The transformation of anisotropic temperature factor coefficients (for the general triclinic case) to principal axes of thermal motion is discussed by Waser,[8] Busing and Levy,[9] and Cruickshank *et al.*[10]

The principal axis transformation is necessary to find the thermal-motion probability ellipsoids discussed in 5.2. The principal axes of the matrix $\mathbf{M}^{-1}$ in (5.3.6) are the vectors $\mathbf{y}_1$, $\mathbf{y}_2$, $\mathbf{y}_3$ for which the inner vector product $(\mathbf{y}_i, \mathbf{y}_i)$ has a stationary value subject to the constraint

$$(\mathbf{y}_i, \mathbf{M}^{-1}\mathbf{y}_i) = 1 , \qquad i = 1, 2, 3 . \tag{5.4.1}$$

For the general triclinic crystal system this means that the quadratic form $\mathbf{y}^T\mathbf{G}^{-1}\mathbf{y}$ has a stationary value subjected to the constraint

$$\mathbf{y}^T\mathbf{G}^{-1}\mathbf{M}^{-1}\mathbf{y} = 1 , \tag{5.4.2}$$

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[8] J. Waser, *Acta Cryst.* **8**, 731 (1955).

[9] W. R. Busing and H. A. Levy, *Acta Cryst.* 11, 450 (1958).

[10] D. W. J. Cruickshank *et al.*, p. 74 in *Computing Methods and the Phase Problem in X-Ray Crystal Analysis*, ed. by R. Pepinsky, J. M. Robertson, and J. C. Speakman, Pergamon, New York, 1961.

where G^{-1} is the metric tensor with components $e_i \cdot e_j$ and $e_i \cdot e_j$ is the scalar vector product of two of the three unit cell vectors. Introducing the Lagrange multiplier $1/\lambda$ leads to

$$\left[G^{-1} - \frac{1}{\lambda_i} M^{-1}\right] y_i = 0 \qquad (i = 1,2,3); \tag{5.4.3}$$

premultiplying by M yields

$$\left[MG^{-1} - \frac{1}{\lambda_i} I\right] y_i = 0 \qquad (i = 1,2,3). \tag{5.4.4}$$

Or we can do some additional rearranging and obtain

$$[GM^{-1} - \lambda_i I] y_i = 0 \qquad (i = 1,2,3). \tag{5.4.5}$$

Equation (5.4.4) is equivalent to one of the results derived by Busing and Levy, except the λ_i obtained here are the reciprocals of their λ_i because we are doing the principal axis transformation on M^{-1} while their formulation performs the transformation on M. The numerical procedure used in OR TEP finds the eigenvalues and eigenvectors of the unsymmetrical matrix MG^{-1} in (5.4.4).

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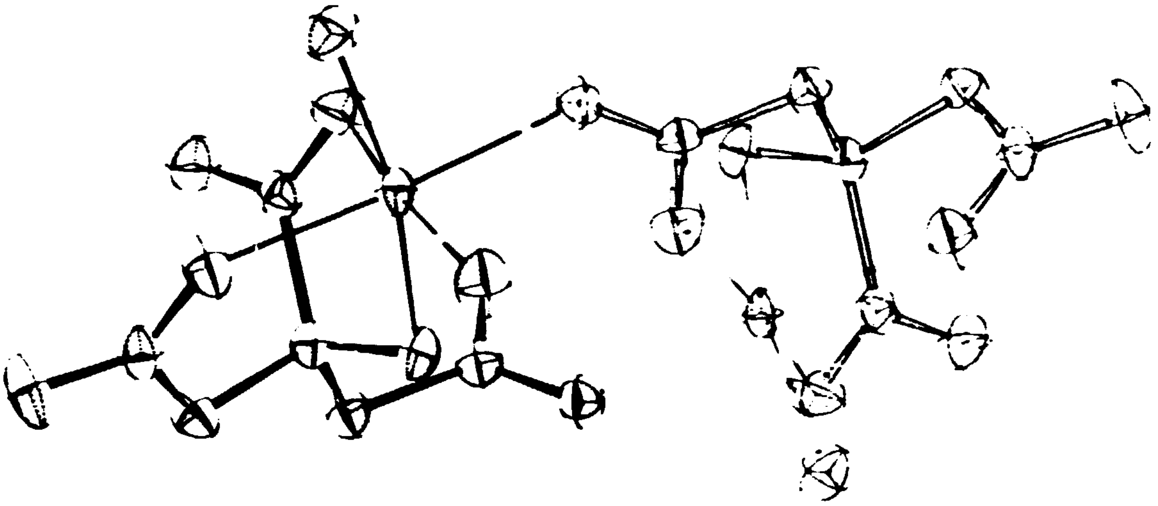

Fig. 6.1. Chelation Pattern Viewed Along a Twofold Screw Axis in the Crystal Structure of Magnesium Citrate Decahydrate. Ellipsoids represent equiprobability surfaces of thermal displacement and contain 65% of the probability distribution.

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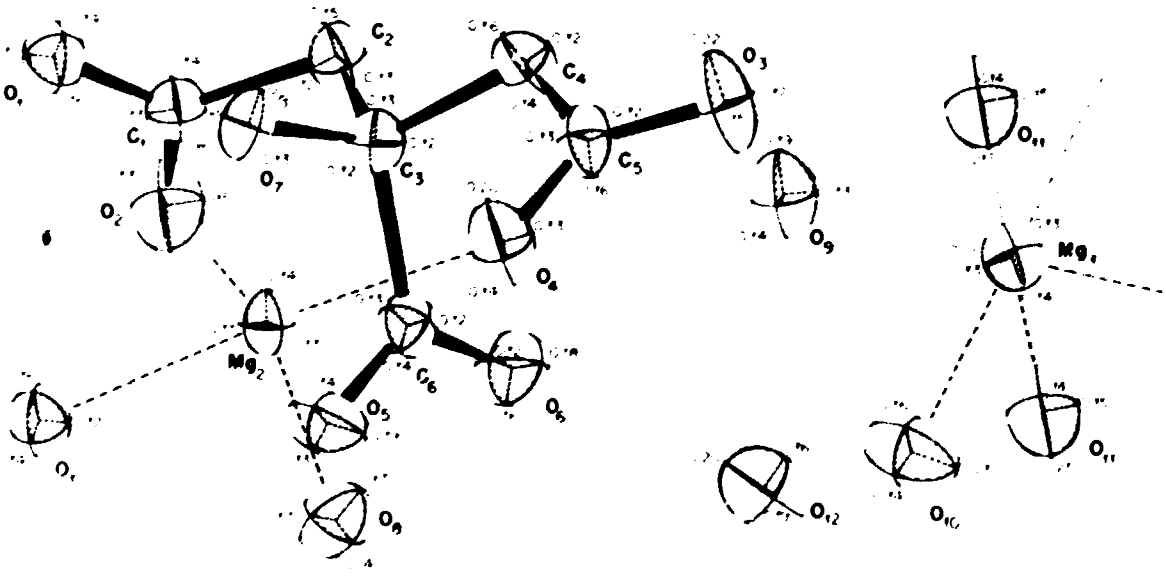

Fig. 6.2. Thermal-Ellipsoid Representation for Magnesium Citrate Decahydrate with Principal Values of RMS Displacement in Angstrom Units. Ellipsoids enclose 74% probability. Structure is viewed along *b* axis.

6.2 Stereoscopic Drawings of Crystal Structures

6.2.1 Thermal Ellipsoids Derived from Neutron Studies. – Thermal ellipsoids for hydrogen atoms can be derived from neutron diffraction data. Some recent crystal structure results refined from three-dimensional neutron data are shown here as stereoscopic pairs of perspective projections. The thermal ellipsoid for a hydrogen atom is almost always larger than that of the heavier neighbor atom because of zero-point energy.

6.2.1.1 Chloral Hydrate. – Figure 6.6 features two molecules of chloral hydrate[5] related by a center of symmetry. The neighboring hydroxyl groups which are involved in hydrogen bonding to the two molecules are also included.

6.2.1.2 Sugars. – A single molecule of sucrose[6] is shown in Fig. 6.7 with the six-membered glucose ring to the left and the five-membered fructose ring to the right. Two intramolecular hydrogen bonds are drawn between the two moieties. Only one hydroxyl group in the molecule does not form a hydrogen bond; this group has the abnormally large thermal ellipsoid for hydrogen on the left side of the figure.

The thermal motion of a glucose molecule in the α-glucose crystal structure[7] is illustrated by Fig. 6.8. This figure was drawn with OR TEP by G. M. Brown.

6.2.1.3 Lithium Sulphate Monohydrate. – The inorganic structure lithium sulphate monohydrate has been refined with three-dimensional x-ray data by Larson[8] and with three zones of two-dimensional neutron data by Smith and Levy.[9] Figure 6.9 illustrates the characteristic atomic arrangement in that structure. The hydrogen thermal ellipsoids were taken from the neutron analysis and the remainder from the x-ray results. The outstanding feature in this illustration is the large thermal motion of the water molecule, which indicates much looser binding than in the rest of the structure.

6.2.1.4 Potassium Hydrogen Chloromaleate.[10] – This structure contains a centered hydrogen bond. The interatomic bond distances and the surrounding K atoms are also shown in Fig. 6.10, which was drawn with OR TEP by R. D. Ellison and H. A. Levy.

6.2.2 Thermal Ellipsoids Derived from X-Ray Studies. – The examples shown in this section were taken from the literature and from the work of several crystallographers who kindly sent their unpublished results to ORNL to be drawn.

6.2.2.1 Long-Chain Aliphatic Organic Compounds. – Dihydromalvalic acid[11] (cis,D,L-8,9-methyleneheptadecanoic acid) is shown in Fig. 6.11. The thermal motion perpendicular to the chain direction is seen to increase in amplitude toward the nonpolar end of the chain.

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[5] G. M. Brown and H. A. Levy, *Cryst. Struct. Commun.* 2, 107 (1973).

[6] G. M. Brown and H. A. Levy, *Science* 141, 921 (1963).

[7] G. M. Brown and H. A. Levy, *Science* 147, 1038 (1965).

[8] A. C. Larson, *Acta Cryst.* 18, 717 (1965).

[9] H. G. Smith, S. W. Peterson, and H. A. Levy, *J. Chem. Phys.* 48, 5561 (1968).

[10] R. D. Ellison and H. A. Levy, *Acta Cryst.* 19, 260 (1965).

[11] G. A. Jeffrey and M. Sax, *Acta Cryst.* 16, 1196 (1963).

Figure 6.12 illustrates the thermal motion in the triglyceride beta-tricaprin.[12] The two molecules shown are related by a center of symmetry. Again the amplitude of motion perpendicular to the chain increases toward the end of the chain.

6.2.2.2 Copper Chelation Compound. – The chelation pattern in *bis*-(3-amino-1-phenyl-2-butene-1-ono)-Cu(II)[13] is demonstrated in Fig. 6.13. The copper atom is on a symmetry center.

6.2.2.3 Large Biological Molecule. – Harunganin,[14] which is a plant pigment, is shown in Fig. 6.14. The pair of "half atoms" at the upper right is an approximation used in the least-squares refinement to correct for either very large thermal motion or disorder which occurs in that part of the crystal structure. The thermal parameters are somewhat questionable since the structure was not refined to convergence. However, the stereogram does permit the molecular configuration to be readily visualized.

6.2.2.4 Abnormal Motion in Cr(III) Acetylacetonate. – Dr. Bruno Morosin from Sandia Corporation sent this most unusual example of thermal motion. Cr(III) acetylacetonate[15] has three acetylacetonate ligands arranged to form an octahedral coordination of oxygens about the Cr atom, as shown in Fig. 6.15. One of the ligands displays very large thermal anisotropy. When a molecular packing diagram such as Fig. 6.16 is viewed, the large displacements are seen to be parallel to the **b** crystal axis. It appears that sheets of these ligands are either disordered or undergoing longitudinal vibration. Morosin has evidence from other diffraction experiments which supports the hypothesis that it is a thermal vibration phenomenon and not static disorder in the crystal.

6.2.3 Crystal Structure Packing Diagrams. – It is often desirable to illustrate the way that molecules pack together in a crystal structure. Sometimes thermal motion can be interpreted on this basis, as was done in 6.2.2.4. In other instances one may be more interested in visualizing the general packing geometry of the crystal structure. Stereograms are very useful for both applications.

6.2.3.1 Potassium Hydrogen Chloromaleate. – A molecule of this structure[10] is shown in Fig. 6.10. Packing diagrams were also drawn by Ellison and Levy and are reproduced here. Figure 6.17 shows the packing of anions about the two types of potassium ions. One coordination polyhedron is an irregular octahedron of oxygen atoms. The other is an irregular 14-hedron having six oxygen atoms and four chlorine atoms at its vertices. Figure 6.18 is a different view of the packing with a larger area included.

6.2.3.2 Packing Diagrams for Inorganic Structures. – The reader may have noticed that most of the illustrations are of organic structures. The reason is that organic molecules are easy to draw. Considerably more planning is required to produce an informative illustration of an inorganic structure.

An approach which is fairly successful is the following:

1. Draw a preliminary stereogram of the contents of a box which encloses somewhat more than one unit cell. Bonds should be drawn in accordance with known interatomic distance ranges. The dimensions

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[12] A. J. Mabis and L. H. Jensen, *Abstracts ACA Meeting, Bozeman, Montana*, F-9 (1964) and L. H. Jensen, private communication, 1964.

[13] G. E. Gurr, *Acta Cryst.* B24, 1511 (1968) and private communication, 1964.

[14] R. A. Alden, G. H. Stout, J. Kraut, and D. F. High, *Acta Cryst.* 17, 109 (1964).

[15] B. Morosin, *Acta Cryst.* 19, 131 (1965) and B. Morosin, private communication, 1964.

for this drawing may be such that the plot can be viewed directly with a stereoscope without photographic reduction.

2. While viewing the preliminary stereogram, pick out the basic structural units and decide on a grouping of these units for the desired figure.

3. Describe the intended subject with whichever technique is the most convenient and draw the new figure. Figure 6.19, potassium perxenate nonahydrate,[16] is an example of an illustration planned in this way. This figure was drawn by J. H. Burns at ORNL.

6.2.3.3 Illustrations of the Contents of a Unit Cell. – A favorite method used by crystallographers is to draw a unit cell outline and the cell contents within that outline. Figure 6.20, which is a stereogram showing lithium α-monodeuteroglycolate,[17] is of this nature. The molecules were kept intact rather than cut off at the cell outline.

6.3 Helical Structures

OR TEP has certain features which facilitate the drawing of nonintegral helical screw models such as those discussed in the field of molecular biology. The Pauling, Corey, and Branson alpha-helix model[18] for protein structure is an example. Figure 6.21 shows the modification of this structure which is present in the synthetic polypeptide poly-L-alanine.[19]

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[16] A. Zalkin, J. D. Forrester, D. H. Templeton, S. M. Williamson, and C. W. Koch, *J. Am. Chem. Soc.* **86**, 3569 (1964).

[17] C. K. Johnson, E. J. Gabe, M. R. Taylor, and I. A. Rose, *J. Am. Chem. Soc.* **87**, 1802 (1965).

[18] L. Pauling, R. B. Corey, and H. R. Branson, *Proc. Natl. Acad. Sci. U.S.* **37**, 235 (1951).

[19] A. Elliott and B. R. Malcolm, *Proc. Roy. Soc. London* **A 249**, 30 (1959).

6. EXAMPLES OF ILLUSTRATIONS THAT HAVE BEEN PRODUCED WITH OR TEP

Most of the drawings reproduced here were made while OR TEP was under development. Consequently, certain details in the figures are not the same as those produced with the present version of the program. In particular, the lines of shading in the ellipsoid "open octant" are now always evenly spaced.

6.1 Nonstereoscopic Drawings Showing Thermal Motion

The figures in this section have the viewpoint at infinity (parallel projection).

6.1.1 Comparison of Graphical Representations of Thermal Motion. – Figure 6.1 shows the chelation pattern of two citrate molecules related by a twofold screw axis in the crystal structure of magnesium citrate decahydrate.[1] One molecule has "transparent ellipsoids" and the other has "opaque, plugged ellipsoids." Bond types 1, 3, and 4 (see 3.3.9) are illustrated. Note that certain bonds terminate at the ellipsoid boundary while others intersect the ellipsoid. These variables are under the user's control and can be used to advantage for special effects.

Figure 6.2 is another drawing of magnesium citrate decahydrate with the rms magnitudes of displacement along principal axes indicated around the equiprobability thermal ellipsoids.

Figure 6.3 illustrates the same figure with the thermal-motion representation mentioned by Waser,[2] in which the thermal motion is portrayed by a fourth-degree surface generated by a radius vector with length proportional to the rms component of displacement in the direction of the radius vector. The characteristic peanut shape of this fourth-degree surface is most apparent for atom O_3.

The thermal ellipsoid seems to be the preferred representation, and the present version of OR TEP will draw ellipsoids only.

6.1.2 Thermal Ellipsoids Derived from Independent Sets of Diffraction Data. – Figures 6.4(*a*) and (*b*) show the thermal ellipsoids for potassium dihydrogen isocitrate[3] obtained from two independent sets of three-dimensional x-ray data (copper K_α data and chromium K_α data). Figure 6.4(*a*) is presumably a better representation since it is based on a much larger number of measurements. In fact, it is rather surprising that the thermal-motion figures are so similar, considering the limited number of data obtainable with chromium radiation.

6.1.3 Thermal Motion in Molecules Not Related by Crystallographic Symmetry. – Myo-inositol[4] has two molecules in its crystallographic asymmetric unit. Figures 6.5(*a*) and 6.5(*b*) permit a comparison of the two sets of thermal ellipsoids in identical molecular orientations. The hydrogen bonds to neighboring atoms are also indicated. The similarity between the two ellipsoid sets is readily apparent.

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[1] C. K. Johnson, *Acta Cryst.* **18**, 1004 (1965).

[2] J. Waser, *Acta Cryst.* **8**, 731 (1955).

[3] D. van der Helm, J. P. Glusker, C. K. Johnson, J. A. Minkin, N. E. Burow, and A. L. Patterson, *Acta Cryst.* B-24, 578 (1968).

[4] I. N. Rabinowitz and J. Kraut, *Acta Cryst.* **17**, 159 (1964).

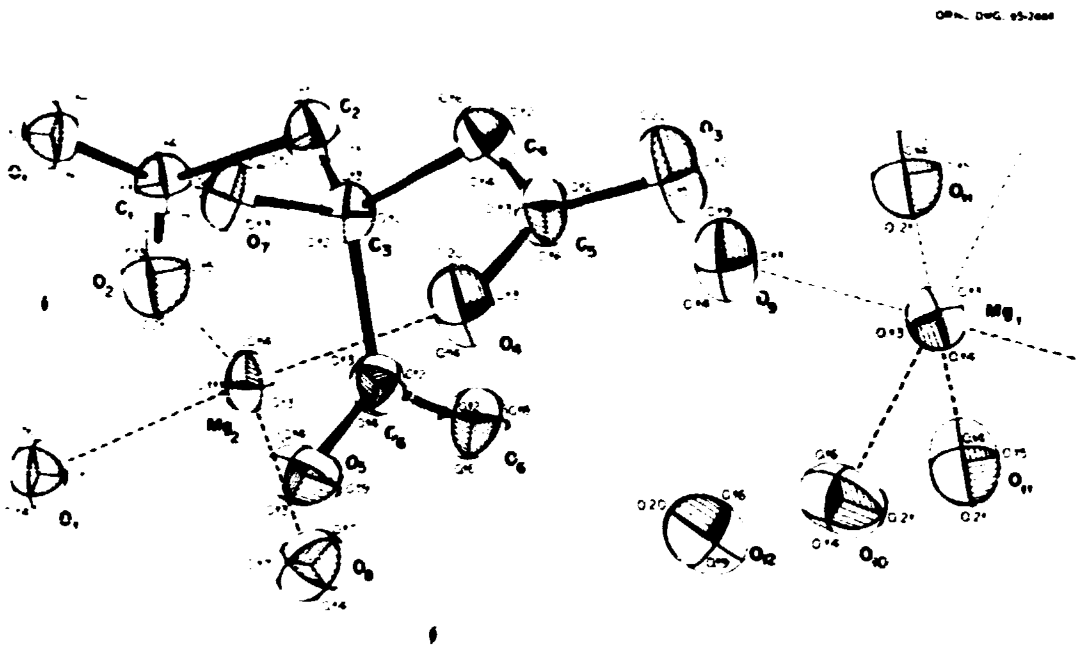

Fig. 6.3. Peanut-Shaped RMS Thermal-Displacement Figure Representation for Magnesium Citrate Decahydrate. Principal values of rms displacement in Angstrom units are indicated around the displacement figures, which are drawn at double scale. Same view of structure as shown in Fig. 6.2.

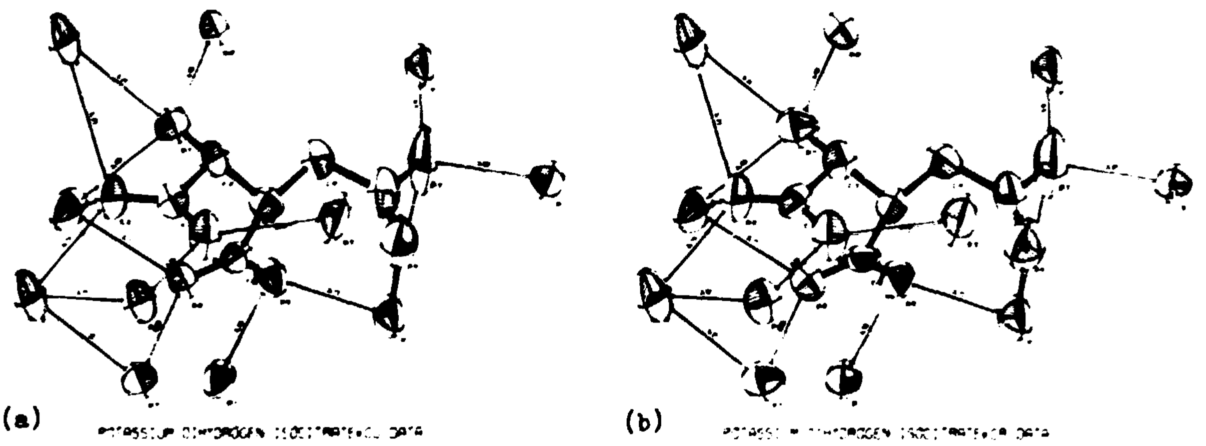

Fig. 6.4. Potassium Dihydrogen Isocitrate with Thermal Ellipsoids Scaled to Include 74% Probability. (*a*) Results obtained from 1350 three-dimensional copper K_α data (disagreement factor 6.5%). (*b*) Results obtained from 340 three-dimensional chromium K_α data (disagreement factor 2.2%). Note: This is *not* a stereo pair.

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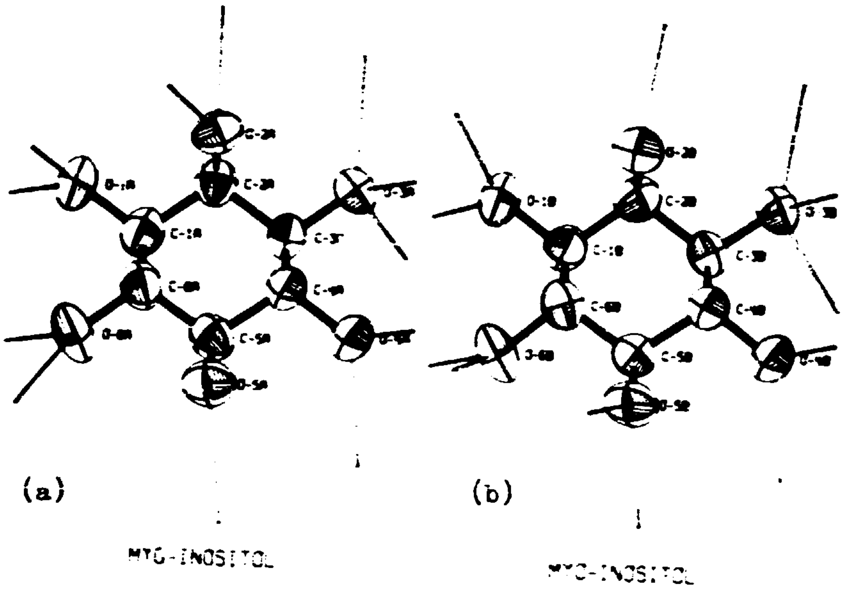

Fig. 6.5. Comparison of Thermal Ellipsoids in the Two Crystallographically Independent Molecules of Myo-Inositol (6.5a and 6.5b). Hydrogen bonding is shown, since this might influence the thermal motion. Ellipsoids are scaled to include 74% probability. Note: This is not a stereo pair.

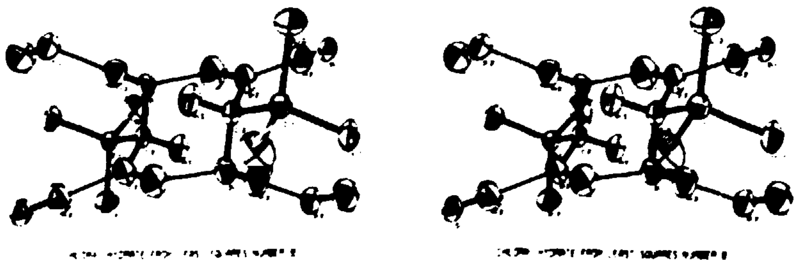

Fig. 6.6. Stereogram (Stereoscopic Pair of Perspective Projections) of Chloral Hydrate Viewed Along the Reciprocal Axis a^*. Two molecules are shown related by a center of symmetry, with the hydrogen bonds connecting them together and to other molecules. Ellipsoids are scaled to include 48% probability.

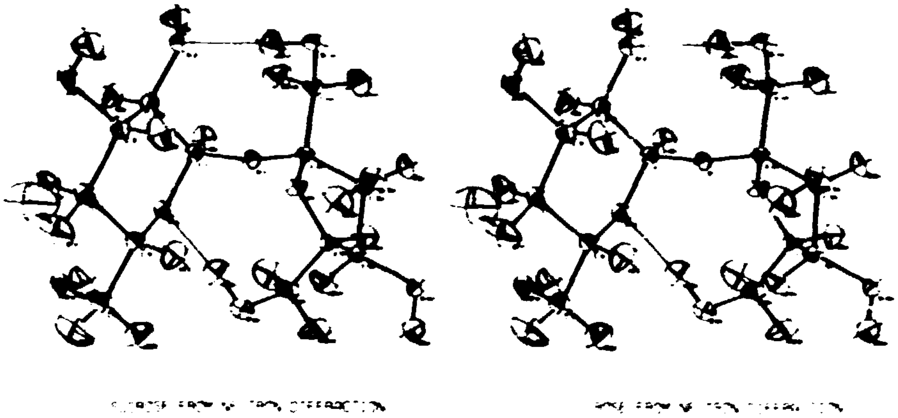

Fig. 6.7. Stereogram Showing the Sucrose Molecule with Thermal Ellipsoids Scaled to Enclose 50% Probability.

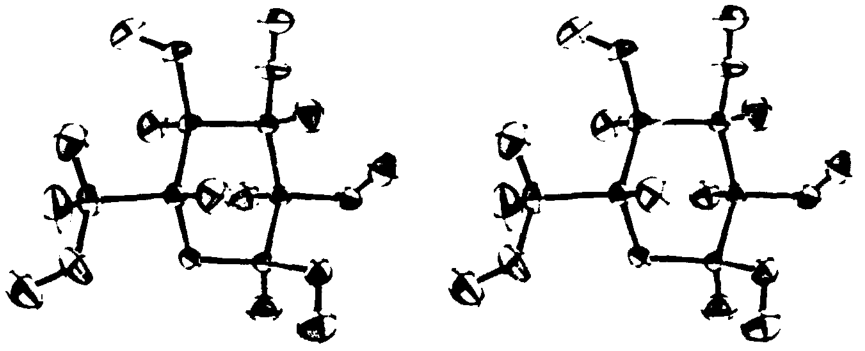

Fig. 6.8. A Molecule of Glucose with Thermal Ellipsoids Scaled to Enclose 50% Probability.

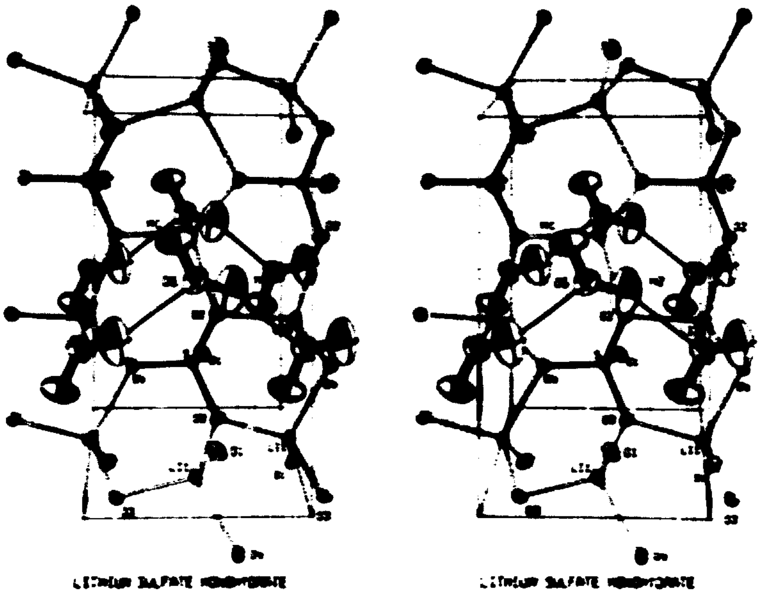

Fig. 6.9. Lithium Sulphate Monohydrate. The lithium ions and sulphate ions are coordinated into a compact network. The structure is viewed along the reciprocal a* axis. The ellipsoids are scaled to enclose 20% probability.

Fig. 6.10. Potassium Hydrogen Chloromaleate. The chloromaleate ion is viewed normal to its own plane. The thermal ellipsoids enclose 50% probability.

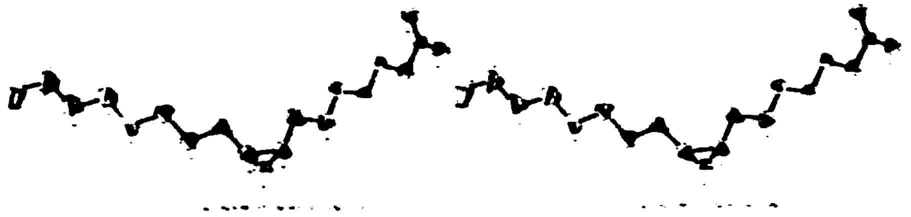

Fig. 6.11. A Molecule of Dihydromalvalic Acid with Thermal Ellipsoids Scaled to Enclose 40% Probability.

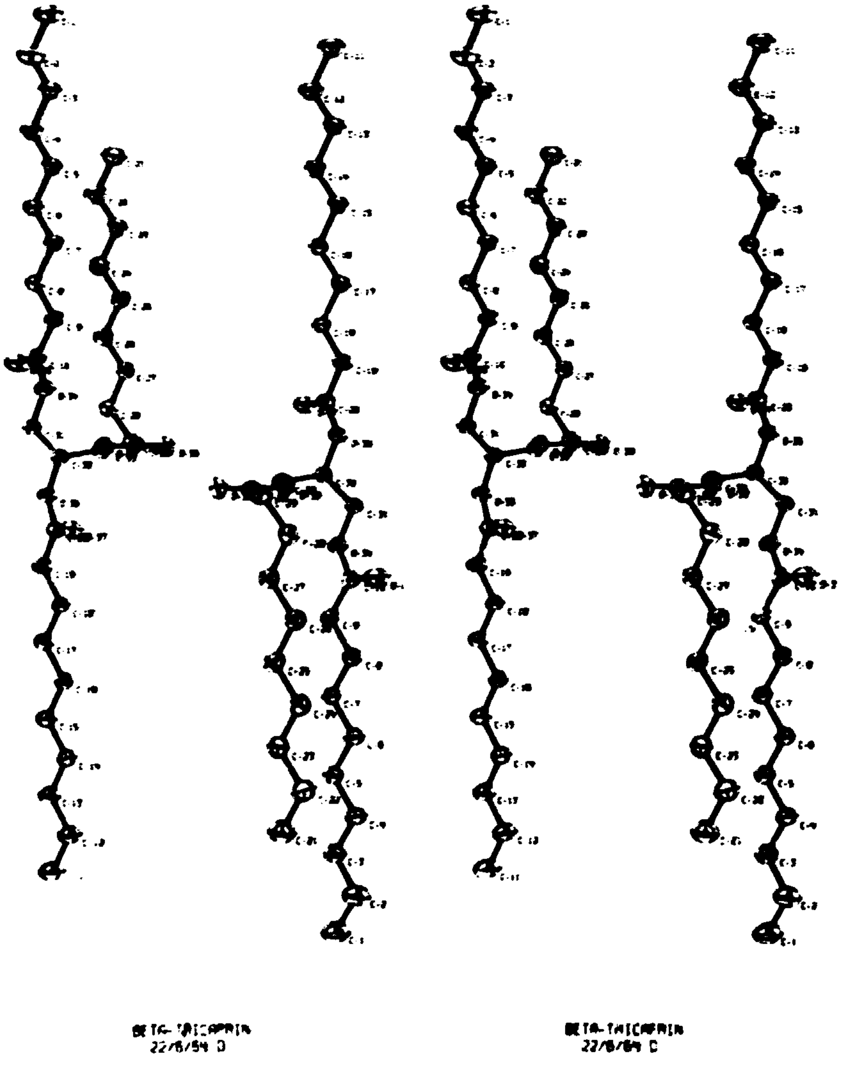

Fig. 6.12. Two Molecules of Beta-Tricaprin Related by a Center of Symmetry. The thermal ellipsoids are scaled to include 30% probability.

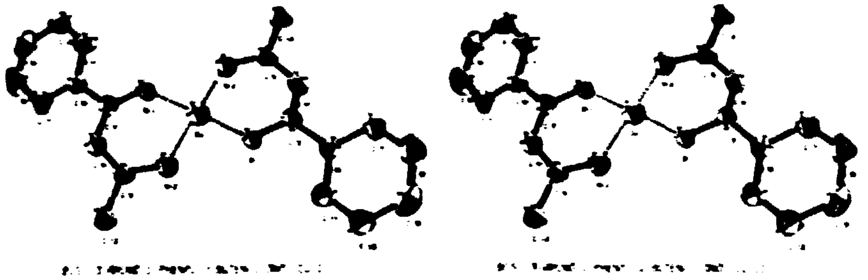

Fig. 6.13. Chelation Complex of *Bis*-(3-amino-1-phenyl-2-butene-1-ono)-Cu(II) with Thermal Ellipsoids Scaled to Include 50% Probability.

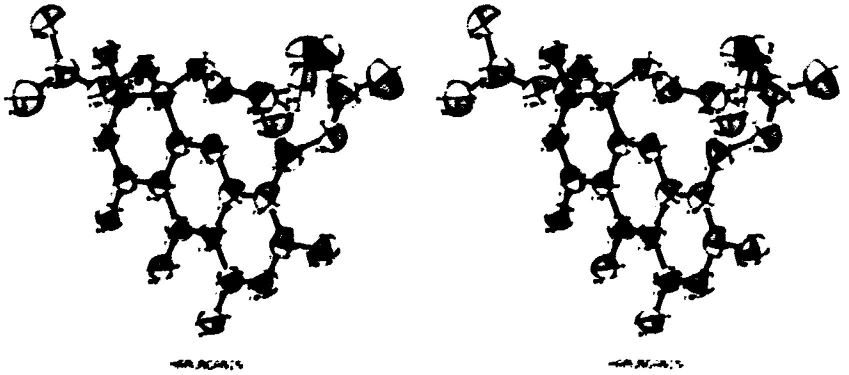

Fig. 6.14. A Molecule of the Plant Pigment Harunganin with Thermal Ellipsoids Scaled to Include 40% Probability.

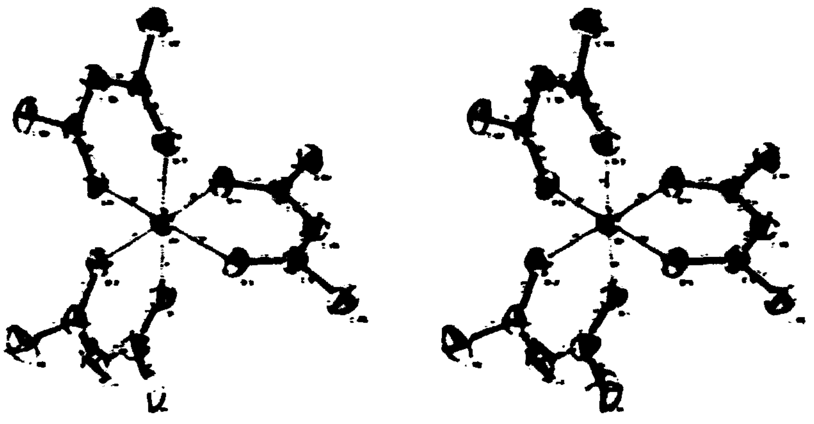

Fig. 6.15. A Unit of *Tris*-acetylacetonatochromium(III) Viewed Along its Threefold Axis of Chemical Symmetry. The thermal ellipsoids are scaled to enclose 20% probability.

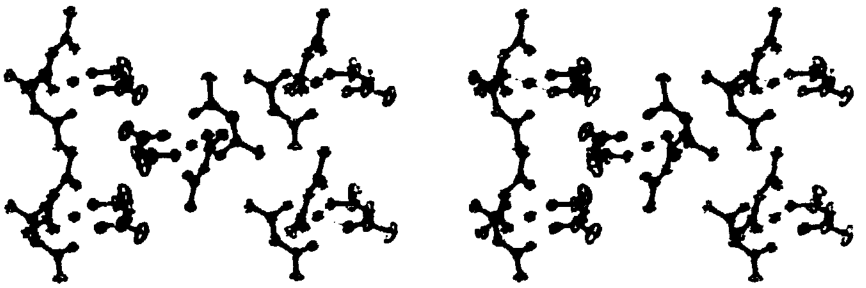

Fig. 6.16. Packing Diagrams for *Tris*-acetylacetonatochromium(III) Viewed Along the Reciprocal Axis c^*. Thermal ellipsoids are scaled to enclose 20% probability.

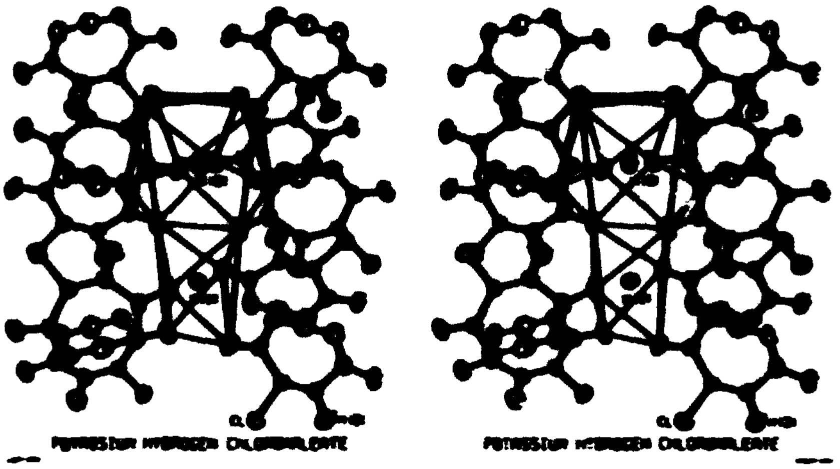

Fig. 6.17. Packing of Chloromaleate Ions Around the Potassium Ions in Potassium Hydrogen Chloromaleate. The edges of the coordination polyhedra are shown. View is nearly along the *c* axis. Thermal ellipsoids are scaled to contain 50% probability.

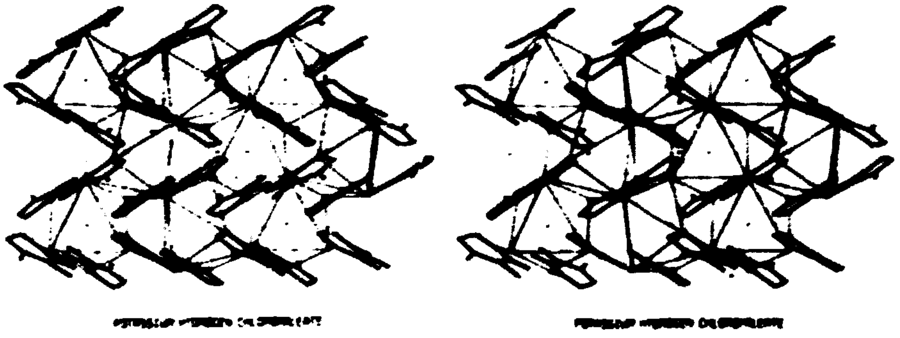

Fig. 6.18. Packing Diagrams for Potassium Hydrogen Chloromaleate. Atoms are represented as small circles. The edges of the coordination polyhedra around the potassium ions are shown. View is nearly along the *a* axis.

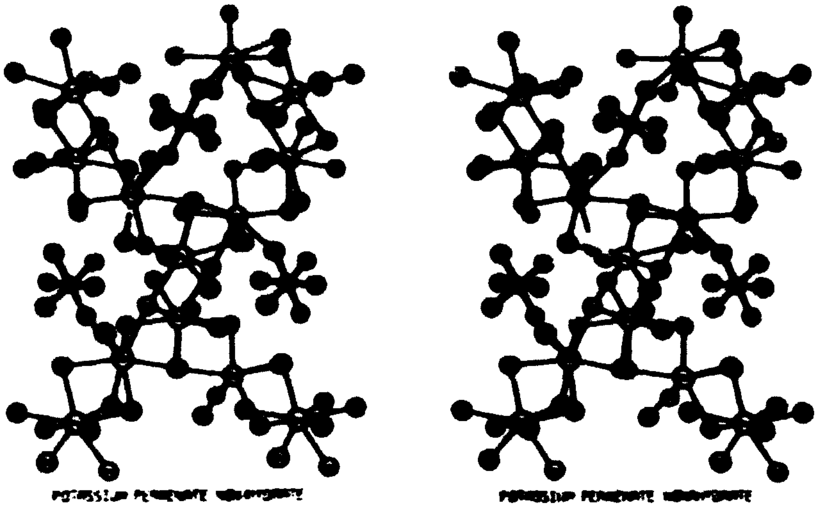

Fig. 6.19. Packing Diagram for Potassium Perxenate 9-Hydrate, Illustrating the Network of Highly Hydrated Potassium Ions Surrounding Perxenate Ions. The view is parallel to the *a* axis. Another layer, related to the present one by a twofold screw axis along *a*, is needed to complete the structure.

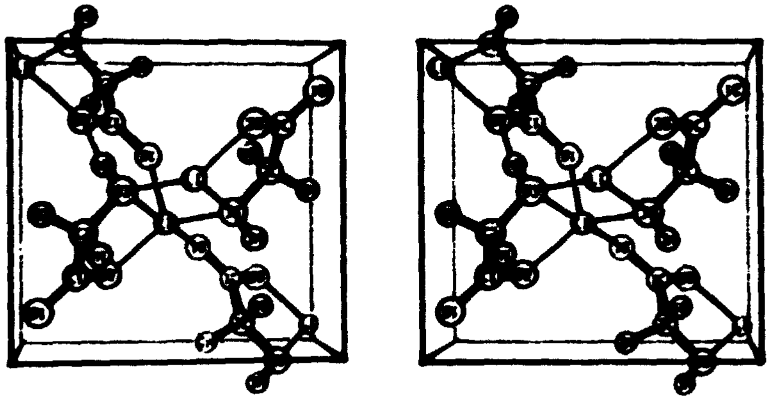

Fig. 6.20. A Stereogram Showing the Unit-Cell Contents of Anhydrous Li α-monodeuteroglycolate. The unique monoclinic *b* axis points up in the page and the mean *c* axis out from the page.

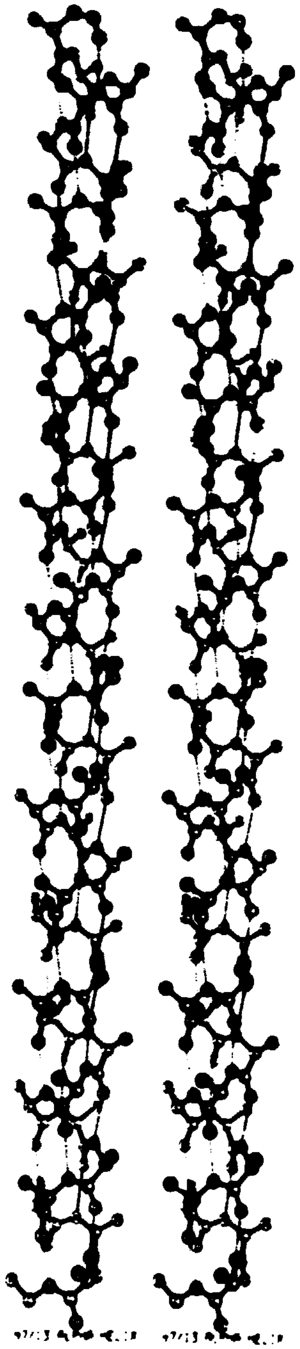

Fig. 6.21. A Stereoscopic Pair of Perspective Projections Showing the Alpha-Helix Which Is Present in Poly-L-Alanine. There are 47 amino-acid residues in 13 turns of the helix. Stereo viewing is accomplished by placing a sheet of cardboard between the helices.

7. FORTRAN LISTING OF OR TEP-II

```
C     TOTAL NUMBER OF CARDS INCLUDING DATA FOR EXAMPLE IS 4705
C     ***** OAK RIDGE THERMAL ELLIPSOID PLOT PROGRAM *****
C     ***** ORTEP-II / IBM-360 / FEB 1971 / INSTRUCTIONS IN ORNL-3794 **
C     ***** OPTIONAL OVERLAP FEATURE ADDED TO ORTEP IN FEBRUARY 1971 ***
C     ***** CURRENT EXAMPLE CARDS ILLUSTRATE USE OF OVERLAP FEATURE *****
C     ***** IN BRIEF, INSTRUCTION 511 MAY BE USED JUST BEFORE EACH
C     ***** DRAWING TO STORE THE PROJECTED ATOMS, TYPE 3 TRAILER CARDS
C     ***** WITH INSTR 511 CAUSES PROJECTED BONDS ALSO TO BE STORED
C     ***** MAXIMUM NUMBER OF STORED BONDS IS 599.  IN GENERAL, JUST USE
C     ***** THE SAME TYPE 2 TRAILER CARDS USED BY THE 802/812 INSTR. ***
C     ***** COLS 10-18 ON 511 INST CARD SPECIFIES OVERLAP MARGIN(OVMRGN)
C     *****        0        OVMRGN = MAX(0.035 OR SQRT(SCAL1)*0.030)
C     *****     1 OR -1     OVMRGN = 0.0
C     *****   .GT.0,.LT.1  OVMRGN = ACTUAL VALUE GIVEN (INCHES) *****
C     ***** ALL OVERLAP INFORMATION IS DESTROYED BY INSTR. 501-510
C     ***** IF THE COMPUTER STORAGE AVAILABLE IS EXCEEDED BY THIS FEATURE
C     ***** SUBROUTINES LAP500, LAP700, LAP800, LAPDRW, LAPAP AND LAPCON
C     ***** MAY BE REMOVED AND REPLACED BY THE FOLLOWING 4 DUMMIES
C     SUBROUTINE LAP500(NTYPE)
C     RETURN
C     END
C     SUBROUTINE LAP700(NA,ICQ)
C     RETURN
C     END
C     SUBROUTINE LAP800(NA1,NA2,ICQ)
C     RETURN
C     END
C     SUBROUTINE LAPDRW(T,NPTN,NCQ)
C     RETURN
C     END
      REAL*8 CHEM
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(146),CONT(5),D(3,110)
      DIMENSION DA(3,3),DP(2,110),EV(3,146),FS(3,3,80),KD(5,40),ORGN(3)
      DIMENSION P(3,146),PA(3,3,146),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3)
      DIMENSION BRS(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,96)
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)
      DIMENSION XLNG(3),XO(3),XT(3)
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D
      COMMON DA,DP,DISP,EDGE,EV,FORM,FS,IN,ITILT,KD,LATM,LTHO,NATOM,NCD
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1
      COMMON SCAL2,SCL,SYMB,TAPED,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT
      LTHO=0
    2 CALL PRIME
C     ***** READ JOB TITLE CARD *****
      READ (IN,4) (TITLE(I),I=1,18)
    4 FORMAT(18A4)
      WRITE (NOUT,6) (TITLE(I),I=1,18)
    5 FORMAT(1H0 10X,18A4)
    6 FORMAT(1H1 10X,18A4)
      CALL PRELIM
      WRITE (NOUT,6) (TITLE(I),I=1,18)
      ISAVE=0
      GO TO 907
    7 ISAVE=0
C     ***** ZERO AIN ARRAY *****
    8 DO 10 J=1,140
   10 AIN(J)=0.
   11 FORMAT(1H0/1X,17H((((( INSTRUCTION,I5,6H ))))))
   12 FORMAT(I3,I6,7F9.0)
   13 FORMAT(I3,I6,7F15.8)
   14 FORMAT(1H 9X,7F15.7)
C     ***** READ NEW INSTRUCTION CARD *****
      NCD=0
      N1=-6
   16 N1=N1+7
      N2=N1+6
      IF(ISAVE)22,18,18
   18 READ (IN,12)IC,NF,(AIN(I),I=N1,N2)
      IF(ISAVE)20,20,20
   20 WRITE (NSR)IC,NF,(AIN(I),I=N1,N2)
      GO TO 24
   22 READ (NSR)IC,NF,(AIN(I),I=N1,N2)
      IF(IC)7,24,24
   24 IF(N1-1)26,26,30
   26 WRITE (NOUT,11)NF
      NF1=NF
      IF(NF1)28,8,30
   28 IF(NF1+2)2,2,1000
   30 WRITE (NOUT,14)(AIN(I),I=N1,N2)
   32 IC=IC+1
      GO TO (90,16,38,50),IC
   33 FORMAT(I3,6X,5I3,8F6.0)
   34 FORMAT(6I3,8F12.5)
   35 FORMAT(1H 11X,5I3,8F11.5)
C     ***** READ FORMAT 2 TRAILER CARDS *****
   38 NCD=NCD+1
      IF(ISAVE)44,40,40
   40 READ (IN,33)IC,(KD(I,NCD),I=1,5),(CD(I,NCD),I=1,8)
      IF(ISAVE)46,46,42
   42 WRITE (NSR)IC,(KD(I,NCD),I=1,5),(CD(I,NCD),I=1,8)
      GO TO 46
   44 READ (NSR)IC,(KD(I,NCD),I=1,5),(CD(I,NCD),I=1,8)
   46 WRITE (NOUT,35)(KD(I,NCD),I=1,5),(CD(I,NCD),I=1,8)
      GO TO 32
C     ***** READ FORMAT 3 TRAILER CARD *****
   50 IF(ISAVE)52,54,54
   52 READ (NSR)(TITLE2(I),I=1,18)
      GO TO 55
   54 READ (IN ,4)(TITLE2(I),I=1,18)
   55 WRITE (NOUT,5)(TITLE2(I),I=1,18)
      IF(ISAVE)90,90,56
   56 WRITE (NSR)(TITLE2(I),I=1,18)
C     ***** EXECUTE INSTRUCTION *****
   90 NJ=NF1/100
      NJ2=NF1-NJ*100
      NJ1=MOD(NJ2,10)
      IF(NJ-12)98,92,92
   92 CALL SPARE(NF1)
      IF(NG)96,8,96
   96 CALL ERPNT(0.,NF1)
      GO TO 8
C     ******BRANCH TABLE FOR FUNCTION TYPES*******
   98 GO TO(100,200,300,400,500,600,700,800,900,1000,1100),NJ
C     *******STRUCTURE ANALYSIS FUNCTIONS*******
  100 GO TO (101,101,104,104,101,101,90),NJ2
  101 CALL ATABC
      GO TO 8
C     ***** ANISOTROPIC TEMP FACTOR OUTPUT *****
  104 DO 160 I=1,NATOM
      IF(MOD(I,10)-1)130,110,130
  110 WRITE (NOUT,6) (TITLE(J),J=1,18)
      WRITE (NOUT,129)
  129 FORMAT(1H0 10X,9HATOM(I),16HRMS DISPLACEMENT,31HUNIT VECTORS, BASED
     1 ON DIRECT SYSTEM,30HPROBABILITY COVARIANCE MATRIX)
  130 T1=55501.+FLOAT(I)*100000.
      CALL PAXES(T1,-1)
      IF(NG)148,154,148
  148 CALL ERPNT(T1,100)
  149 FORMAT(1H0 10X,A6,F10.4,6X,3F12.7,10X,3F12.7)
  154 WRITE (NOUT,149)CHEM(I),RMS(1),(PAC(J,1),J=1,3),(Q(J,1)
     1,J=1,3)
  160 WRITE (NOUT,159)(RMS(K),(PAC(J,K),J=1,3),(Q(J,K),J=1,3)
     1,K=2,3)
  159 FORMAT(1H 16X,F10.4,6X,3F12.7,10X,3F12.7)
      GO TO 8
C     ******PLOTTER INITIALIZE,FRAME ADVANCE,TERMINATE FUNCTIONS*********
  200 CALL F200
      GO TO 8
  300 GO TO (301,302,303,90),NJ2
C     ******PLOT DIMENSIONS*******
  301 IF(AIN(1))321,321,311
  311 XLNG(1)=AIN(1)
  321 IF(AIN(2))341,341,331
  331 XLNG(2)=AIN(2)
  341 IF(AIN(3))361,351,351
  351 VIEW=AIN(3)
  361 IF(AIN(4))381,381,371
  371 BRDR=AIN(4)
  381 WRITE (NOUT,389)XLNG(1),XLNG(2),BRDR
  389 FORMAT(1H0 10X,11HPLOT LIMITSF6.2,3H BYF6.2,15H IN.  INCLUDINGF6.2,
     112H IN. MARGIN)
  391 WRITE (NOUT,399)VIEW
  399 FORMAT(1H 10X,13HVIEW DISTANCEF7.3,7H INCHES)
      GO TO 8
C     *******LEGEND ROTATION*******
  302 THETA=AIN(1)
      T1=THETA*.01745329252
      COSTH=COS(T1)
      SINTH=SIN(T1)
      DO 313 J=1,9
```

```
  312 SYMB(J,1)=0.                                                      MAIN1630
      SYMB(1,1)=COSTH                                                   MAIN1640
      SYMB(2,2)=COSTH                                                   MAIN1650
      SYMB(3,3)=1.                                                      MAIN1660
      SYMB(2,1)=SINTH                                                   MAIN1670
      SYMB(1,2)=-SINTH                                                  MAIN1680
      WRITE (NOUT,319) THETA                                            MAIN1690
  319 FORMAT(1H0 10X,46HRECTANGULAR TITLE AND SYMBOL ROTATION IN DEGREESF8.2)MAIN1700
      GO TO 8                                                           MAIN1710
C     ***** RETRACE DISPLACEMENT *****                                  MAIN1720
  301 DISP=ATN(1)                                                       MAIN1730
      WRITE (NOUT,313) DISP                                             MAIN1740
  313 FORMAT(1H0 10X,22HRETRACE DISPLACEMENT =F7.3,5H IN.)              MAIN1750
      GO TO 8                                                           MAIN1760
C     *******ATOM LIST FUNCTIONS*******                                 MAIN1770
  400 GO TO (401,401,401,401,401,401,490, 98, 98,410,                   MAIN1780
     1        401,401,401,401,401,401, 98),NJ2                          MAIN1790
  401 CALL F400                                                         MAIN1800
      GO TO 490                                                         MAIN1810
  410 LATM=0                                                            MAIN1820
      DO 420 I=1,500                                                    MAIN1830
      DO 420 J=1,4                                                      MAIN1840
  420 ATOMS(J,I)=0.                                                     MAIN1850
  490 IF (LATM) 8,8,491                                                 MAIN1860
  491 WRITE (NOUT,499) (ATOMS(1,I),I=1,LATM)                            MAIN1870
  499 FORMAT(1H0 10X,23HCONTENTS OF ATOMS ARRAY/(15X,10F10.0))          MAIN1880
      GO TO 8                                                           MAIN1890
C     *******CARTESIAN COORDINATE SYSTEM FUNCTIONS*******               MAIN1900
  500 CALL F500                                                         MAIN1910
      WRITE  (NOUT,501) (ORGN(J),J=1,3)                                 MAIN1920
  501 FORMAT(1H0,10X,    46HORIGIN FOR PROJECTION AXIS IN CRYSTAL COORD.MAIN1930
     1,3F15.4)                                                          MAIN1940
      IF (NJ2-3) 507,539,506                                            MAIN1950
  506 IF (NJ2-6) 601,507,601                                            MAIN1955
  507 WRITE (NOUT,509)                                                  MAIN1960
      WRITE (NOUT,519) ((REFV(J,I),I=1,3),(AAREV(J,I),I=1,3),J          MAIN1970
     1=1,3)                                                             MAIN1980
      GO TO 4                                                           MAIN1990
  509 FORMAT(1H0 10X, 49HORTHONORMAL WORKING VECTORS BASED ON CRYSTAL AXEMAIN2000
     1S 10X,33HPOST-FACTOR TRANSFORMATION MATRIX/ 14X,8HX VECTOR8X,8HY VECMAIN2010
     2TOR8X,8HZ VECTOR)                                                 MAIN2020
  519 FORMAT(1H 10X,3F14.7,8X,3F16.7)                                   MAIN2030
  529 FORMAT(1H0 10X,51HORTHONORMAL REFERENCE VECTORS BASED ON CRYSTAL AXMAIN2040
     1ES 16X,33HPOST-FACTOR TRANSFORMATION MATRIX/14X,8HX VECTOR8X,8HY VEMAIN2050
     2CTOR8X,8HZ VECTOR)                                                MAIN2060
  539 WRITE (NOUT,529)                                                  MAIN2070
      WRITE (NOUT,519) ((REFV(J,I),I=1,3),(AAUDM(J,I),I=1,3),J          MAIN2080
     1=1,3)                                                             MAIN2090
      GO TO 8                                                           MAIN2100
C     *******PLOT CENTERING FUNCTIONS*******                            MAIN2110
  601 CALL F600                                                         MAIN2120
  603 WRITE (NOUT,609) XO(1),XO(2),SCAL1,SCAL2                          MAIN2130
  609 FORMAT(1H0 10X,33HORIGIN POINT IN PLOTTED COORD.(F6.2,2H ,F6.2,8H )MAIN2140
     1 IN.  / 11X,15HOVERALL SCALE =F6.3,32H INCH/ANGSTROM ELLIPSOID SCAMAIN2150
     2LE =F6.3)                                                         MAIN2160
      GO TO 301                                                         MAIN2170
C     *******ELLIPSOID AND SYMBOL PLOT FUNCTIONS*******                 MAIN2180
C     *********FILL OUT DETAILS FOR SPECIAL MODELS*********             MAIN2190
  700 GO TO (701,702,703,704,705,709),NJ                                MAIN2200
  701 ATN(1)=4.                                                         MAIN2210
      GO TO 703                                                         MAIN2220
  702 ATN(1)=0.                                                         MAIN2230
  703 ATN(3)=4.                                                         MAIN2240
      ATN(2)=0.                                                         MAIN2250
      ATN(4)=0.                                                         MAIN2260
      GO TO 709                                                         MAIN2270
  704 ATN(3)=3.                                                         MAIN2280
      ATN(2)=-5.                                                        MAIN2290
      GO TO 706                                                         MAIN2300
  705 ATN(1)=1.                                                         MAIN2310
      ATN(2)=0.                                                         MAIN2320
  706 ATN(3)=3.                                                         MAIN2330
      ATN(4)=5.                                                         MAIN2340
  709 CALL F700                                                         MAIN2350
      GO TO 8                                                           MAIN2360
C     *********BOND FUNCTIONS*******                                    MAIN2370
  800 CALL F800                                                         MAIN2380
      GO TO 8                                                           MAIN2390
C     *******TITLE FUNCTIONS*******                                     MAIN2400
  900 CALL F900                                                         MAIN2410
      GO TO 8                                                           MAIN2420
C     *******CELL OUTLINE FUNCTIONS*******                              MAIN2430
 1000 CALL F1000                                                        MAIN2440
      GO TO 8                                                           MAIN2450
```

```
C     *******SAVE SEQUENCE FUNCTIONS*******                             MAIN2460
 1100 IF (NJ2-2) 1101,1102,1103                                         MAIN2470
 1101 ISAVE=1                                                           MAIN2480
      GO TO 1104                                                        MAIN2490
 1102 ISAVE=0                                                           MAIN2500
      J=-1                                                              MAIN2510
      END FILE NSR                                                      MAIN2520
      GO TO 1104                                                        MAIN2530
 1103 ISAVE=-1                                                          MAIN2540
 1104 REWIND NSR                                                        MAIN2550
      GO TO 8                                                           MAIN2560
C     ***** TERMINATE PLOTTER TAPE IF NECESSARY *****                   MAIN2570
 3000 IF (LTWO) 3005,3010,3005                                          MAIN2580
 3005 ATN(1)=-.000001                                                   MAIN2590
      ATN(2)= 0.0                                                       MAIN2600
      NJ2=2                                                             MAIN2610
      CALL F200                                                         MAIN2620
 3010 CALL EXIT                                                         MAIN2630
      STOP                                                              MAIN2640
      END                                                               MAIN2650


      FUNCTION ARCCOS(X)                                                ARCC  10
C     ARCCOS(X) IN DEGREES                                              ARCC  20
      IF (1.0-ABS(X)) 1,2,2                                             ARCC  30
    1 X=SIGN(1.0,X)                                                     ARCC  40
    2 IF (X) 3,4,5                                                      ARCC  50
    3 ARCCOS=180.0+ATAN(SQRT(1.0-X*X)/X)*57.29577951                    ARCC  60
      GO TO 6                                                           ARCC  70
    4 ARCCOS=90.0                                                       ARCC  80
      GO TO 6                                                           ARCC  90
    5 ARCCOS=ATAN (SQRT(1.0-X*X)/X)*57.29577951                         ARCC 100
    6 RETURN                                                            ARCC 110
      END                                                               ARCC 120


      SUBROUTINE ATOM(QA,X)                                             ATOM  10
C     ATOM COORDINATE SUBROUTINE                                        ATOM  20
      DIMENSION X(3),Z(3)                                               ATOM  30
      REAL*8 CHEM                                                       ATOM  40
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAUDM(3,3),AID(3,3),AIN(100)    ATOM  50
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(100),CONT(5),D(3,110)ATOM  60
      DIMENSION DA(3,3),DP(2,110),EV(3,100),FS(3,3,96),FD(5,10),ORGN(3) ATOM  70
      DIMENSION P(3,100),PA(3,3,100),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) ATOM  80
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,96)   ATOM  90
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   ATOM 100
      DIMENSION XLNG(3),XO(3),XT(3)                                     ATOM 110
      COMMON A,AA,AAREV,AAUDM,AID,AIN,ATOMS,BB,BBCK,CD,CHEM,CONT,D      ATOM 120
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,I[illegible]IT,KD,LATM,LTWO,NATOM,NCD ATOM 130
      COMMON NJ,NJ2,NOUT,NPA,NSTR,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1ATOM 140
      COMMON SCAL2,SCL,SYMB,TAPED,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   ATOM 150
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                ATOM 160
      N=QA/100000.0                                                     ATOM 170
      IF (N) 109,109,117                                                ATOM 180
  109 X(1)=0.0                                                          ATOM 190
      X(2)=0.0                                                          ATOM 200
      X(3)=0.0                                                          ATOM 210
      GO TO 125                                                         ATOM 220
  117 IF (N-NATOM) 119,119,501                                          ATOM 230
  501 NG=5                                                              ATOM 240
      GO TO 125                                                         ATOM 250
  119 DO 121 J=1,3                                                      ATOM 260
  121 X(J)=P(J,N)                                                       ATOM 270
  125 TA=ABS(QA)                                                        ATOM 280
      KSYM=AMOD(TA,100000.0)                                            ATOM 290
      KT=KSYM/100                                                       ATOM 300
      KS=KSYM-100*KT                                                    ATOM 310
      IF (KS-NSTR) 203,203,503                                          ATOM 320
  503 NG=4                                                              ATOM 330
      GO TO 125                                                         ATOM 340
  203 IF (KS) 503,205,211                                               ATOM 350
  205 Z(1)=X(1)                                                         ATOM 360
      Z(2)=X(2)                                                         ATOM 370
      Z(3)=X(3)                                                         ATOM 380
      GO TO 311                                                         ATOM 390
  211 DO 223 K=1,3                                                      ATOM 400
      Z(K)=TS(K,KS)                                                     ATOM 410
      DO 223 J=1,3                                                      ATOM 420
  223 Z(K)=Z(K)+FS(J,K,KS)*X(J)                                         ATOM 430
  311 IF (KT) 503,325,313                                               ATOM 440
  313 IF (KT-555) 317,315,317                                           ATOM 450
  315 KSYM=KS                                                           ATOM 460
      GO TO 325                                                         ATOM 470
  317 K1=KT/100                                                         ATOM 480
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```
      N=NT-100*N1                                                       ATOM 490
      N2=N/10                                                           ATOM 500
      N3=N-10*N2                                                        ATOM 510
      X(1)=X(1)+FLOAT(N1-5)                                             ATOM 520
      X(2)=X(2)+FLOAT(N2-5)                                             ATOM 530
      X(3)=X(3)+FLOAT(N3-5)                                             ATOM 540
  125 RETURN                                                            ATOM 550
      END                                                               ATOM 560


      SUBROUTINE ALEQ(A1,X,B1,JJJ)                                      ALEQ  10
C     ***** SOLUTION OF MATRIX EQUATION AX=B FOR X *****                ALEQ  20
C     ***** USES METHOD OF TRIANGULAR ELIMINATION *****                 ALEQ  30
C     ***** B AND X HAVE DIMENSIONS (3,JJJ),A IS ALWAYS (3,3)           ALEQ  40
C     ***** TO INVERT A MAKE B 3 BY 3 IDENTITY MATRIX *****             ALEQ  50
      DIMENSION A1(3,3),A(3,3),B(3,3),B1(3,3),X(3,3)                    ALEQ  60
      NV=JJJ                                                            ALEQ  70
C     ***** TRANSFER DATA *****                                         ALEQ  80
      DO 2 I=1,3                                                        ALEQ  90
      DO 2 J=1,3                                                        ALEQ 100
      IF(NV-J) 2,1,1                                                    ALEQ 110
    1 B(I,J)=B1(I,J)                                                    ALEQ 120
    2 A(I,J)=A1(I,J)                                                    ALEQ 130
C     ***** TRIANGULARIZE MATRIX A *****                                ALEQ 140
      DO 17 I=1,2                                                       ALEQ 150
      S=0.0                                                             ALEQ 160
      DO 4 J=I,3                                                        ALEQ 170
      R=ABS(A(J,I))                                                     ALEQ 180
      IF(R-S)4,3,3                                                      ALEQ 190
    3 S=R                                                               ALEQ 200
      L=J                                                               ALEQ 210
    4 CONTINUE                                                          ALEQ 220
      IF(L-I)5,10,5                                                     ALEQ 230
    5 DO 6 J=I,3                                                        ALEQ 240
      S=A(I,J)                                                          ALEQ 250
      A(I,J)=A(L,J)                                                     ALEQ 260
    6 A(L,J)=S                                                          ALEQ 270
      DO 8 J=1,NV                                                       ALEQ 280
      S=B(I,J)                                                          ALEQ 290
      B(I,J)=B(L,J)                                                     ALEQ 300
    8 B(L,J)=S                                                          ALEQ 310
   10 TEM=A(I,I)                                                        ALEQ 320
      IF(TEM) 11,17,11                                                  ALEQ 330
   11 IPO=I+1                                                           ALEQ 340
      DO 16 J=IPO,3                                                     ALEQ 350
      IF(A(J,I)) 12,16,12                                               ALEQ 360
   12 S=A(J,I)/TEM                                                      ALEQ 370
      A(J,I)=0.0                                                        ALEQ 380
      DO 13 K=IPO,3                                                     ALEQ 390
   13 A(J,K)=A(J,K)-A(I,K)*S                                            ALEQ 400
      DO 15 K=1,NV                                                      ALEQ 410
   15 B(J,K)=B(J,K)-B(I,K)*S                                            ALEQ 420
   16 CONTINUE                                                          ALEQ 430
   17 CONTINUE                                                          ALEQ 440
C     ***** VERIFY SINGULAR MATRIX *****                                ALEQ 450
      DO 20 I=1,3                                                       ALEQ 460
      IF(A(I,I))20,19,20                                                ALEQ 470
   19 A(I,I)=AMAX1(1.E-25,AMAX1(A(1,1),A(2,2),A(3,3))*1.E-15)           ALEQ 480
   20 CONTINUE                                                          ALEQ 490
      DO 26 K=1,NV                                                      ALEQ 500
      DO 26 I=1,3                                                       ALEQ 510
      N=4-I                                                             ALEQ 520
      M=N+1                                                             ALEQ 530
      TEM=B(N,K)                                                        ALEQ 540
      IF(3-N)23,21,21                                                   ALEQ 550
   21 DO 22 J=M,3                                                       ALEQ 560
   22 TEM=TEM-A(N,J)*B(J,K)                                             ALEQ 570
   23 B(N,K)=TEM/A(N,N)                                                 ALEQ 580
   26 X(N,K)=B(N,K)                                                     ALEQ 590
      RETURN                                                            ALEQ 600
      END                                                               ALEQ 610


      SUBROUTINE AXES(U,V,W,ITYPE)                                      AXES  10
C     ***** SETS THREE ORTHOGONAL VECTORS EACH 1 ANGSTROM LONG *****    AXES  20
C     ***** ITYPE .GT.0 FOR CARTESIAN,.LE.0 FOR TRICLINIC *****         AXES  30
C     *****IABS(ITYPE)=1 W(1)=U,W(2)=(UXV),W(3)=UX(UXV) *****           AXES  40
C     *****IABS(ITYPE)=2 W(1)=U,W(2)=(UXV)XU,W(3)=(UXV) *****           AXES  50
C     ***** ITYPE=0 W(1)=A,W(2)=(AXB)XA,W(3)=(AXB), ABC=CELL VECTORS ***AXES  60
      DIMENSION U(3),V(3),W(3,3),X(3,3)                                 AXES  70
      IT=ITYPE                                                          AXES  80
      IF(IT) 115,105,115                                                AXES  90
  105 U(1)=1.                                                           AXES 100
      U(2)=0.                                                           AXES 110
      U(3)=0.                                                           AXES 120
      V(1)=0.                                                           AXES 130
      V(2)=1.                                                           AXES 140
      V(3)=0.                                                           AXES 150
  115 DO 125 J=1,3                                                      AXES 160
  125 W(J,1)=U(J)                                                       AXES 170
      IF(IABS(IT)-1) 165,135,145                                        AXES 180
  135 CALL NORM(U,V,W(1,3),IT)                                          AXES 190
      CALL NORM(U,W(1,3),W(1,2),IT)                                     AXES 200
      GO TO 155                                                         AXES 210
  145 CALL NORM(U,V,W(1,2),IT)                                          AXES 220
      CALL NORM(W(1,2),U,W(1,3),IT)                                     AXES 230
  155 DO 185 I=1,3                                                      AXES 240
      IF(IT) 165,165,175                                                AXES 250
  165 IC=-1                                                             AXES 260
      GO TO 185                                                         AXES 270
  175 IC=1                                                              AXES 280
  185 CALL UNIT(W(1,I),W(1,I),IC)                                       AXES 290
      RETURN                                                            AXES 300
      END                                                               AXES 310


      SUBROUTINE BOND(K1,K2,ND,DA1,NA2)                                 BOND  10
      DIMENSION D(3,3),E(3,3),X(3,3),Q(3,3),VUE(3)                      BOND  20
      DIMENSION VT(3),V(10,2),A(3),T(3)                                 BOND  30
      REAL*8 CHEM                                                       BOND  40
      DIMENSION A(5),AA(3,3),AARTY(3,3),AAVBK(3,3),AID(3,3),AIN(140)    BOND  50
      DIMENSION ATOMS(6,500),BB(3,3),COD(5,10),CHEM(100),CONT(5),D(3,110)BOND  60
      DIMENSION DA(3,3),DP(2,110),EV(3,165),FS(3,3,80),ID(5,10),NG(10(3)BOND  70
      DIMENSION P(3,165),PA(3,3,165),PAC(3,3),PAT(3,3),Q(3,3),QPPT(3,3) BOND  80
      DIMENSION RES(5),RMS(5),STOR(3,3),TITLE(10),TITLE2(10),TS(3,96)   BOND  90
      DIMENSION V7(3,6),V1(8),V2(3),V3(3),V4(3),V5(3),V6(3),XOUT(3,3)   BOND 100
      DIMENSION XLOM(3),XO(3),XT(3)                                     BOND 110
      COMMON N1,A,AA,AARTY,AAVBK,AID,AIN,ATOMS,BB,BBBB,CD,COLN,CONT,D   BOND 120
      COMMON DA,DP,DISP,DDOT,EV,INDR,FS,IN,ITILT,KD,LATM,LION,NATOM,NG  BOND 130
      COMMON NJ,NJ2,NOUT,NSO,NTIN,NRON,P,PA,PAC,PAT,Q,PSTV,PIN,QMR,SCAL1BOND 140
      COMMON SCAL2,SCL,SYMB,TAPED,THETA,TITLE,TITLE2,TS,V1,V10,V7,V1,V2 BOND 150
      COMMON V3,V4,V5,V6,VOLT,XLOM,XO,XT                                BOND 160
C     ***** OBTAIN ADDITIONAL PARAMETERS *****                          BOND 170
      NA1=0                                                             BOND 180
      DO 105 J=1,20                                                     BOND 190
  105 V(J,1)=0.                                                         BOND 200
      V(1,1)=K1                                                         BOND 210
      V(1,2)=K2                                                         BOND 220
      DO 115 I=1,2                                                      BOND 230
      CALL XYZ(V(1,I),V(4,I),3)                                         BOND 240
      IF(NJ) 125,110,125                                                BOND 250
  110 DO 115 J=1,3                                                      BOND 260
  115 V(J+6,I)=XT(J)                                                    BOND 270
      N=V(1,I)/100000.                                                  BOND 280
      K=V(1,I)-FLOAT(N)*100000.                                         BOND 290
      CALL [illegible](V(4,I),V(7,I))                                   BOND 300
      IF(NDAT-NDDDD.[illegible]) 120,125,120                            BOND 310
  120 NA=19                                                             BOND 320
  125 NA=1                                                              BOND 330
      WRITE (NOUT,130)CHEM(N),K,L,(V(J,I),J=2,9)                        BOND 340
      CALL [illegible](V(1,I),NA0)                                      BOND 350
      GO TO 115                                                         BOND 360
  120 IF(NJ2-10) 110,115,115                                            BOND 370
  110 WRITE (NOUT,130)CHEM(N),K,L,(V(J,I),J=2,9)                        BOND 380
  115 CONTINUE                                                          BOND 390
  130 FORMAT(1H 10X,A6,I4 [illegible] (I1,1H,I5,0H) [illegible] /F9.2,3X,3F9.4,3X,3F9.4)BOND 400
      IF(NA1)999,100,999                                                BOND 410
  103 CALL DIFF(V(7,1),V(7,2),VT)                                       BOND 420
      DIST=SQRT(VMV(VT,AA,VT))                                          BOND 430
      IF(MOD(NJ2,10)-1) 102,102,102                                     BOND 440
  102 NATO=NJ2/10                                                       BOND 450
      CALL [illegible](V(2,1),V(1,1),NAT,MOD(IFIX(V(1,1)/100000.),10),5,,*BOND 460
     11)                                                                BOND 470
      CALL [illegible](V(2,2),V(1,2),NAT,MOD(IFIX(V(1,2)/100000.),10),5,,*BOND 480
     12)                                                                BOND 490
      GO TO 170                                                         BOND 500
  101 NDDU=ND(5,NB)                                                     BOND 510
      IF(NDDU) 104,100,104                                              BOND 520
  104 NDDD=0                                                            BOND 530
      GO TO 108                                                         BOND 540
  105 NDDD=-NDDU                                                        BOND 550
  108 NDDP-120/100000?                                                  BOND 560
C     ***** FIND DIFFERENT ATOM PUT IN POSITION ONE *****               BOND 570
  148 IF(V(1,1)) 152,150,152                                            BOND 580
  150 V(12,1)=1.                                                        BOND 590
      V(12,2)=1.                                                        BOND 600
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      IF(N12-2) [illegible]                                      [illegible]
  [illegible] IF [illegible]                                     [illegible]
C     ***** [illegible] *****                                    [illegible]
  [illegible] CALL DRAW[illegible]                               [illegible]
      DO [illegible]                                             [illegible]
  [illegible] CALL DRAW[illegible]                               [illegible]
      DO [illegible]                                             [illegible]
  [illegible] CALL DRAW[illegible]                               [illegible]
      CALL DRAW[illegible]                                       [illegible]
C     ***** [illegible] *****                                    [illegible]
  [illegible] [illegible]                                        [illegible]
  [illegible] [illegible]                                        [illegible]
      IF [illegible]                                             [illegible]
  [illegible] CALL DRAW[illegible]                               [illegible]
      CALL DRAW[illegible]                                       [illegible]
      [illegible]                                                [illegible]
      IF [illegible]                                             [illegible]
  [illegible] CALL DRAW[illegible]                               [illegible]
      CALL DRAW[illegible]                                       [illegible]
      GO TO [illegible]                                          [illegible]
  [illegible] [illegible]                                        [illegible]
      [illegible]                                                [illegible]
      IF [illegible]                                             [illegible]
C     ***** PERSPECTIVE [illegible] *****                        [illegible]
C     ***** [illegible] *****                                    [illegible]
  [illegible] [illegible]                                        [illegible]
      CALL [illegible]                                           [illegible]
      CALL [illegible]                                           [illegible]
      CALL [illegible]                                           [illegible]
      DO [illegible]                                             [illegible]
      [illegible]                                                [illegible]
      IF [illegible]                                             [illegible]
  [illegible] IF [illegible]                                     [illegible]
  [illegible] IF [illegible]                                     [illegible]
  [illegible] [illegible]                                        [illegible]
      [illegible]                                                [illegible]
  [illegible] DO [illegible]                                     [illegible]
      [illegible]                                                [illegible]
  [illegible] [illegible]                                        [illegible]
      DO [illegible]                                             [illegible]
  [illegible] [illegible]                                        [illegible]
C     ***** CHECK [illegible] *****                              [illegible]
      IF [illegible]                                             [illegible]
  [illegible] CALL [illegible]                                   [illegible]
      [illegible]                                                [illegible]
      [illegible]                                                [illegible]
      [illegible]                                                [illegible]
      [illegible]                                                [illegible]
      [illegible]                                                [illegible]
      IF [illegible]                                             [illegible]
  [illegible] [illegible]                                        [illegible]
      [illegible]                                                [illegible]
      [illegible]                                                [illegible]
      [illegible]                                                [illegible]
      [illegible]                                                [illegible]
      [illegible]                                                [illegible]
      [illegible]                                                [illegible]
      [illegible]                                                [illegible]
      [illegible]                                                [illegible]
      CALL [illegible]                                           [illegible]
  [illegible] [illegible]                                        [illegible]
      IF [illegible]                                             [illegible]
  [illegible] WRITE [illegible]                                  [illegible]
  [illegible] FORMAT [illegible]                                 [illegible]
  [illegible] RETURN                                             [illegible]
      END                                                        [illegible]

      SUBROUTINE DIFV(X,Y,Z)                                     DIFV   10
C     VECTOR - VECTOR                                            DIFV   20
C     Z(I)=X(I)-Y(I)                                             DIFV   30
      DIMENSION X(3),Y(3),Z(3)                                   DIFV   40
      DO 111 I=1,3                                               DIFV   50
  111 Z(I)=X(I)-Y(I)                                             DIFV   60
      RETURN                                                     DIFV   70
      END                                                        DIFV   80

      SUBROUTINE DRAW([illegible])                               DRAW   10
      DIMENSION [illegible]                                      DRAW   20
      [illegible] CARD                                           DRAW   30
      DIMENSION [illegible]                                      DRAW   40
      DIMENSION [illegible]                                      DRAW   50
      DIMENSION [illegible]                                      DRAW   60
      DIMENSION [illegible]                                      DRAW   70
      DIMENSION [illegible]                                      DRAW   80
      DIMENSION [illegible]                                      DRAW   90
      DIMENSION [illegible]                                      DRAW  100
      COMMON [illegible]                                         DRAW  110
      COMMON [illegible]                                         DRAW  120
      COMMON [illegible]                                         DRAW  130
      COMMON [illegible]                                         DRAW  140
      COMMON [illegible]                                         DRAW  150
      [illegible]                                                DRAW  160
      [illegible]                                                DRAW  170
      IF [illegible]                                             DRAW  180
C     ***** ROTATE AND PERSPECTIVE TITLE *****                   DRAW  190
  [illegible] [illegible]                                        DRAW  200
      DO [illegible]                                             DRAW  210
  [illegible] [illegible]                                        DRAW  220
      DO [illegible]                                             DRAW  230
  [illegible] [illegible]                                        DRAW  240
      CALL PLTTT(X,Y)                                            DRAW  250
C     ***** CHECK BOUNDS *****                                   DRAW  260
  [illegible] DO [illegible]                                     DRAW  270
      IF [illegible]                                             DRAW  280
  [illegible] [illegible]                                        DRAW  290
  [illegible] IF [illegible]                                     DRAW  300
  [illegible] [illegible]                                        DRAW  310
  [illegible] CONTINUE                                           DRAW  320
C     ***** CHECK FOR OVERLAP *****                              DRAW  330
      [illegible]                                                DRAW  340
      CALL [illegible]                                           DRAW  350
      IF [illegible]                                             DRAW  360
C     ***** CALL PLOTTING ROUTINE IF NO OVERLAPPING ELEMENTS ARE [illegible] DRAW  370
  [illegible] CALL [illegible]                                   DRAW  380
  [illegible] RETURN                                             DRAW  390
      END                                                        DRAW  400

      SUBROUTINE EIGEN (N,VALU,VECT)                             EIGN   10
C     ***** EIGENVALUES AND EIGENVECTORS OF 3X3 MATRIX *****     EIGN   20
      DIMENSION [illegible]                                      EIGN   30
      COMMON [illegible]                                         EIGN   40
C     ***** STATEMENT FUNCTION *****                             EIGN   50
      [illegible]                                                EIGN   60
C     ***** START OF PROGRAM *****                               EIGN   70
      [illegible]                                                EIGN   80
      SIGMA=0.                                                   EIGN   90
      DO [illegible]                                             EIGN  100
      DO [illegible]                                             EIGN  110
      [illegible]                                                EIGN  120
      [illegible]                                                EIGN  130
  [illegible] [illegible]                                        EIGN  140
C     ***** CHECK FOR NULL MATRIX *****                          EIGN  150
      IF [illegible]                                             EIGN  160
  [illegible] SIGMA=SQRT(SIGMA)                                  EIGN  170
C     ***** FORM CHARACTERISTIC EQUATION *****                   EIGN  180
      [illegible]                                                EIGN  190
      [illegible]                                                EIGN  200
     [illegible]                                                 EIGN  210
      [illegible]                                                EIGN  220
     [illegible]                                                 EIGN  230
C     ***** FIRST PART OF [illegible] *****                      EIGN  240
      [illegible]                                                EIGN  250
      [illegible]                                                EIGN  260
      [illegible]                                                EIGN  270
      [illegible]                                                EIGN  280
      IF [illegible]                                             EIGN  290
  [illegible] IF [illegible]                                     EIGN  300
  [illegible] [illegible]                                        EIGN  310
      GO TO [illegible]                                          EIGN  320
  [illegible] [illegible]                                        EIGN  330
      [illegible]                                                EIGN  340
      IF [illegible]                                             EIGN  350
  [illegible] [illegible]                                        EIGN  360
C     ***** [illegible].GT.0.AND.[illegible].GT.0. *****         EIGN  370
  [illegible] [illegible]                                        EIGN  380
      DO [illegible]                                             EIGN  390
  [illegible] IF [illegible]                                     EIGN  400
  [illegible] [illegible]                                        EIGN  410
      GO TO 200                                                  EIGN  420
  [illegible] [illegible]                                        EIGN  430
  200 [illegible]                                                EIGN  440
      [illegible]                                                EIGN  450
      [illegible]                                                EIGN  460
      IF [illegible]                                             EIGN  470
  [illegible] IF [illegible]                                     EIGN  480
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  210 IF (ABS(TEM/VOLD)-ERROR) 250,250,225                             EIGR 490
  225 CONTINUE                                                         EIGR 500
C     ***** DID NOT CONVERGE, SET ERROR INDICATOR *****                EIGR 510
  230 NG=6                                                             EIGR 520
      GO TO 400                                                        EIGR 530
C     ***** STORE FIRST ROOT *****                                     EIGR 540
  250 U(3)=VNEW                                                        EIGR 550
C     ***** DEFLATE *****                                              EIGR 560
      C1=B2-VNEW                                                       EIGR 570
      C0=B1+C1*VNEW                                                    EIGR 580
C     ***** SOLVE QUADRATIC *****                                      EIGR 590
      TEM=C1*C1-4.*C0                                                  EIGR 600
      IF(TEM) 255,265,260                                              EIGR 610
C     ***** IGNORE IMAGINARY COMPONENT OF COMPLEX ROOT *****           EIGR 620
  255 TEM=0.                                                           EIGR 630
      GO TO 265                                                        EIGR 640
  260 TEM=SQRT(TEM)                                                    EIGR 650
  265 U(1)=.5*(C1-TEM)                                                 EIGR 660
      U(2)=.5*(C1+TEM)                                                 EIGR 670
C     ***** SORT ROOTS *****                                           EIGR 680
      DO 275 J=1,2                                                     EIGR 690
      IF(U(J)-U(3)) 275,275,270                                        EIGR 700
  270 TEM=U(J)                                                         EIGR 710
      U(J)=U(3)                                                        EIGR 720
      U(3)=TEM                                                         EIGR 730
  275 CONTINUE                                                         EIGR 740
      LLL=-2                                                           EIGR 750
      DO 375 III=1,2                                                   EIGR 760
C     ***** CHECK FOR MULTIPLE ROOTS *****                             EIGR 770
      TEM=ERROR*100.                                                   EIGR 780
      NG=0                                                             EIGR 790
      L=1                                                              EIGR 800
      DO 305 I=1,2                                                     EIGR 810
      IF(U(I+1)-U(I)-TEM) 300,300,290                                  EIGR 820
  290 IF(U(I)) 295,305,295                                             EIGR 830
  295 IF(ABS((U(I+1)-U(I))/U(I))-TEM) 300,300,305                      EIGR 840
  300 L=L+1                                                            EIGR 850
      NG=NG-2*I                                                        EIGR 860
  305 CONTINUE                                                         EIGR 870
      IF(LLL-L) 309,400,400                                            EIGR 880
  309 LLL=L                                                            EIGR 890
C     ***** EIGENVECTOR ROUTINE *****                                  EIGR 900
      DO 375 II=1,3                                                    EIGR 910
      T1=U(II)                                                         EIGR 920
      IF(L) 315,310,322                                                EIGR 930
C     ***** TWO VECTORS NULL FOR DOUBLE ROOT *****                     EIGR 940
  310 IF(NG+5-II) 315,322,315                                          EIGR 950
C     ***** ALL VECTORS NULL FOR TRIPLE ROOT *****                     EIGR 960
  315 DO 320 J=1,3                                                     EIGR 970
  320 VECT(J,II)=0.0                                                   EIGR 980
      GO TO 375                                                        EIGR 990
  322 DO 325 J=1,3                                                     EIGR1000
  325 A(J,J)=B(J,J)-T1                                                 EIGR1010
      SMAX=0.0                                                         EIGR1020
      DO 355 I=1,3                                                     EIGR1030
      I1=1                                                             EIGR1040
      IF(I-3) 335,335,340                                              EIGR1050
  335 I1=I+1                                                           EIGR1060
  340 B(I,1)=A(I,2)*A(I1,3)-A(I,3)*A(I1,2)                             EIGR1070
      B(I,2)=A(I,3)*A(I1,1)-A(I,1)*A(I1,3)                             EIGR1080
      B(I,3)=A(I,1)*A(I1,2)-A(I,2)*A(I1,1)                             EIGR1090
      TEM=B(I,1)**2+B(I,2)**2+B(I,3)**2                                EIGR1100
      IF(TEM-SMAX) 355,355,350                                         EIGR1110
  350 SMAX=TEM                                                         EIGR1120
      IMAX=I                                                           EIGR1130
  355 CONTINUE                                                         EIGR1140
      IF(SMAX) 353,353,360                                             EIGR1150
  353 NG=7                                                             EIGR1160
      GO TO 375                                                        EIGR1170
  360 SMAX=SQRT(SMAX)                                                  EIGR1180
      DO 365 J=1,3                                                     EIGR1190
  365 V(J)=B(IMAX,J)/SMAX                                              EIGR1200
C     ***** REFINE EIGENVECTOR *****                                   EIGR1210
      CALL AXSQU(A,T,V,1)                                              EIGR1220
      TEM=AMAX1(ABS(V(1)),ABS(V(2)),ABS(V(3)))                         EIGR1230
      DO 370 J=1,3                                                     EIGR1240
  370 V(J)=V(J)/TEM                                                    EIGR1250
      CALL UNIT(V,VECT(1,II),1)                                        EIGR1260
C     ***** REFINE EIGENVALUE *****                                    EIGR1270
      T1=VMV(VECT(1,II),B,VECT(1,II))                                  EIGR1280
      U(II)=T1                                                         EIGR1290
  375 VALU(II)=T1                                                      EIGR1300
  400 RETURN                                                           EIGR1310
      END                                                              EIGR1320
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      SUBROUTINE ERPNT(T1,M)                                           ERPN  10
      REAL*8 CHEM                                                      ERPN  20
      DIMENSION A(9),AA(3,3),AADEV(3,3),AAVER(3,3),AID(3,3),AIN(100)   ERPN  30
      DIMENSION ATOMS(8,500),BD(3,3),CD(8,10),CHEM(166),CONT(5),D(3,110) ERPN  40
      DIMENSION DA(3,3),DP(2,130),EV(3,166),PS(3,3,40),KD(5,10),ORGN(3) ERPN  50
      DIMENSION P(3,166),PA(3,3,166),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) ERPN  60
      DIMENSION RES(8),RMS(5),STND(3,3),TITLE(18),TITLE2(18),TS(3,40)  ERPN  70
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),UNKV(3,3)  ERPN  80
      DIMENSION XLMG(3),XO(3),XT(3)                                    ERPN  90
      COMMON NG,A,AA,AADEV,AAVER,AID,AIN,ATOMS,BD,BUSR,CD,CHEM,CONT,D  ERPN 100
      COMMON DA,DP,DISP,EDGE,EV,FORM,PS,ID,ITILT,KD,LATM,LTMO,NATOM,NCD ERPN 110
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1ERPN 120
      COMMON SCAL2,SCL,STND,TAPED,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2  ERPN 130
      COMMON V3,V4,V5,V6,UNKV,XLMG,XO,XT                               ERPN 140
      WRITE (NOUT,115) NG,T1,M                                         ERPN 150
  115 FORMAT(1H0 10X,10HFAULT NG =I3,F10.0,I6/1H )                     ERPN 160
      NG=0                                                             ERPN 170
      RETURN                                                           ERPN 180
      END                                                              ERPN 190


      SUBROUTINE F200                                                  F200  10
      DIMENSION HEADER(4),PLA(3000)                                    F200  20
      DATA HEADER/3*6H      ,4H0   /,ZERO/0.0/                         F200  30
      REAL*8 CHEM                                                      F200  40
      DIMENSION A(9),AA(3,3),AADEV(3,3),AAVER(3,3),AID(3,3),AIN(100)   F200  50
      DIMENSION ATOMS(8,500),BD(3,3),CD(8,10),CHEM(166),CONT(5),D(3,110) F200  60
      DIMENSION DA(3,3),DP(2,130),EV(3,166),PS(3,3,40),KD(5,10),ORGN(3) F200  70
      DIMENSION P(3,166),PA(3,3,166),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) F200  80
      DIMENSION RES(8),RMS(5),STND(3,3),TITLE(18),TITLE2(18),TS(3,40)  F200  90
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),UNKV(3,3)  F200 100
      DIMENSION XLMG(3),XO(3),XT(3)                                    F200 110
      COMMON NG,A,AA,AADEV,AAVER,AID,AIN,ATOMS,BD,BUSR,CD,CHEM,CONT,D  F200 120
      COMMON DA,DP,DISP,EDGE,EV,FORM,PS,ID,ITILT,KD,LATM,LTMO,NATOM,NCD F200 130
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1F200 140
      COMMON SCAL2,SCL,STND,TAPED,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2  F200 150
      COMMON V3,V4,V5,V6,UNKV,XLMG,XO,XT                               F200 160
C     ***** CALCOMP CONTROL *****                                      F200 170
      NJG = NJ2+1                                                      F200 180
      GO TO(260,200,225,205,210,260),NJG                               F200 190
C     ***** INITIATE MECHANICAL CALCOMP PLOTTER (201 INSTRUCTION) ***** F200 200
  200 LTMO = 15                                                        F200 210
      CALL PLOTS(PLA,3000,LTMO)                                        F200 220
      GO TO 260                                                        F200 230
C     ***** INITIATE C.R.T. CALCOMP PLOTTER (203 INSTRUCTION) *****    F200 240
  205 LTMO = -99                                                       F200 250
      CALL JOBNUM(HEADER(1))                                           F200 260
      CALL TDAY(HEADER(2))                                             F200 270
      CALL CRT(PLA,3000,HEADER,0)                                      F200 280
C     ***** SET C.R.T. X,Y ORIGIN AND BEAM INTENSITY BASELINE *****    F200 290
      IZ = AIN(3)                                                      F200 300
      CALL CRT(AIN(1),AIN(2),IZ,1)                                     F200 310
      GO TO 215                                                        F200 320
C     ***** RESET BEAM INTENSITY (204 INSTRUCTION) *****               F200 330
  210 IZ = AIN(3)                                                      F200 340
      IF(IZ) 215,215,220                                               F200 350
  215 IZ = 10                                                          F200 360
  220 CALL CRT(ZERO,ZERO,IZ,7)                                         F200 370
      GO TO 260                                                        F200 380
C     ***** TERMINATE THE PLOT AND ADVANCE PLOTTER (202 INSTRUCTION) ***F200 390
  225 IF(LTMO) 235,260,230                                             F200 400
  230 CALL PLOT(AIN(1),AIN(2),-3)                                      F200 410
      GO TO 265                                                        F200 420
C     ***** THE FOLLOWING ARE FOR CRT FILM ADVANCE ETC. *****          F200 430
  235 IF(AIN(1)) 245,240,250                                           F200 440
C     ***** ADD BLACK ADDRESS BUT DO NOT ADVANCE CRT FILM *****        F200 450
  240 ID = 1000                                                        F200 460
      GO TO 255                                                        F200 470
C     ***** ADVANCE CRT FILM AND CLOSE OUTPUT TAPE FILE ****           F200 480
  245 ID = 9000                                                        F200 490
      GO TO 255                                                        F200 500
C     ***** ADD BLOCK ADDRESS AND ADVANCE CRT FILM *****               F200 510
  250 ID = 8000                                                        F200 520
C     ***** IDENTIFICATION TITLE FRAME BETWEEN PLOTS *****             F200 530
      CALL CRT(ZERO,ZERO,10,2)                                         F200 540
      CALL SYMBOL(0.2,9.0,0.25,TITLE(1),90.,72)                        F200 550
  255 CALL CRT(ZERO,ZERO,ID,7)                                         F200 560
  260 RETURN                                                           F200 570
      END                                                              F200 580


      SUBROUTINE F400                                                  F400  10
C     ***** ATOM LIST FUNCTIONS *****                                  F400  20
      REAL*8 CHEM                                                      F400  30
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      DIMENSION A(9),AA(3,3),AAREV(3,3),AAUBH(3,3),AIO(3,3),AIN(140)      P400  40
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHRN(144),CONT(5),D(3,130) P400  50
      DIMENSION DA(3,3),DP(2,130),DV(3,144),FS(3,3,40),ED(5,10),ORGN(3)  P400  60
      DIMENSION P(3,144),PA(3,3,144),PAC(3,5),PAT(3,3),Q(3,3),RTPV(3,3)  P400  70
      DIMENSION RES(8),RMS(5),STHD(3,3),TITLE(10),TITLE2(10),TS(3,40)    P400  80
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),UNIV(3,3)    P400  90
      DIMENSION XLNG(3),XO(3),XT(3)                                      P400 100
      COMMON NG,A,AA,AAREV,AAUBH,AIO,AIN,ATOMS,BB,BROH,CD,CHIN,CONT,D    P400 110
      COMMON DA,DP,DISP,EDGE,EV,FORM,FS,ID,ITILT,KD,LATN,LTNC,NATOM,NCD P400 120
      COMMON NJ,NJ2,NOUT,NSD,NSYM,ORGN,P,PA,PAC,PAT,Q,RTPV,RES,RMS,SCAL1P400 130
      COMMON SCAL2,SCL,STHD,TAPED,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2    P400 140
      COMMON V3,V4,V5,V6,UNIV,XLNG,XO,XT                                 P400 150
      NG=0                                                               P400 160
      IF(LATN)402,402,400                                                P400 170
  400 DO 401 I=1,LATN                                                    P400 180
  401 CALL ATOS(ATOMS(1,I),ATOMS(2,I))                                   P400 190
  402 IF(MOD(NJ2,10)-1)499,404,403                                       P400 200
  403 CALL STARC                                                         P400 210
      GO TO 499                                                          P400 220
C     ***** STORES (401) OR REMOVES (411) RUNS OF ATOMS *****            P400 230
C     ***** RUN HIERARCHY = ATOM NO./SYM/ A/B/C TRANS. *****             P400 240
  404 II=1                                                               P400 250
C     ***** FIND RUNS IN AIN ARRAY *****                                 P400 260
  405 T1=AIN(II)                                                         P400 270
      IF(T1)410,410,420                                                  P400 280
  410 II=II+1                                                            P400 290
      IF(140-II)499,405,405                                              P400 300
  420 JJ=II                                                              P400 310
C     ***** SET INITIAL RUN VALUES *****                                 P400 320
      N1=T1/100000.                                                      P400 330
      N2=AMOD(T1,100.)                                                   P400 340
      N5=AMOD(T1/100.,1000.)                                             P400 350
      IF(N5)422,422,423                                                  P400 360
  422 N5=999                                                             P400 370
  423 N3=N5/100                                                          P400 380
      N4=MOD(N5/10,10)                                                   P400 390
      N5=MOD(N5,10)                                                      P400 400
  425 JJ=JJ+1                                                            P400 410
      IF(140-JJ)435,430,430                                              P400 420
  430 T2=-AIN(JJ)                                                        P400 430
      IF(T2)435,425,440                                                  P400 440
  435 II=JJ-1                                                            P400 450
C     ***** SET TERMINAL VALUES FOR DEGENERATE RUN *****                 P400 460
      M1=N1                                                              P400 470
      M2=N2                                                              P400 480
      M3=N3                                                              P400 490
      M4=N4                                                              P400 500
      M5=N5                                                              P400 510
      GO TO 450                                                          P400 520
  440 II=JJ                                                              P400 530
C     ***** SET TERMINAL RUN VALUES *****                                P400 540
      M1=T2/100000.                                                      P400 550
      M2=AMOD(T2,100.)                                                   P400 560
      M5=AMOD(T2/100.,1000.)                                             P400 570
      IF(M5)445,445,446                                                  P400 580
  445 M5=999                                                             P400 590
  446 M3=M5/100                                                          P400 600
      M4=MOD(M5/10,10)                                                   P400 610
      M5=MOD(M5,10)                                                      P400 620
C     ***** LOOP THROUGH ALL RUNS *****                                  P400 630
  450 DO 490 L5=N5,M5                                                    P400 640
      DO 490 L4=N4,M4                                                    P400 650
      DO 490 L3=N3,M3                                                    P400 660
      DO 490 L2=N2,M2                                                    P400 670
      DO 490 L1=N1,M1                                                    P400 680
      V1(1)=FLOAT(L1)*100000.+FLOAT(L3*10000+L4*1000+L5*100+L2)          P400 690
      CALL ATOM(V1(1),V1(2))                                             P400 700
      IF(NG)455,458,455                                                  P400 710
  455 CALL ERPRT(V1(1),401)                                              P400 720
      GO TO 490                                                          P400 730
  458 CALL STOD                                                          P400 740
  490 CONTINUE                                                           P400 750
      GO TO 410                                                          P400 760
  499 RETURN                                                             P400 770
      END                                                                P400 780

      SUBROUTINE P500                                                    P50   10
      DIMENSION RR(3,3),V(3,4)                                           P50.  20
      REAL*8 CHEM                                                        P500  30
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAUBH(3,3),AIO(3,3),AIN(140)      P500  40
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHRN(144),CONT(5),D(3,130) P500  50
      DIMENSION DA(3,3),DP(2,130),DV(3,144),FS(3,3,40),ED(5,10),ORGN(3)  P500  60
      DIMENSION P(3,144),PA(3,3,144),PAC(3,5),PAT(3,3),Q(3,3),RTPV(3,3)  P500  70
      DIMENSION RES(8),RMS(5),STHD(3,3),TITLE(10),TITLE2(10),TS(3,40)    P500  80
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),UNIV(3,3)    P500  90
      DIMENSION XLNG(3),XO(3),XT(3)                                      P500 100
      COMMON NG,A,AA,AAREV,AAUBH,AIO,AIN,ATOMS,BB,BRDP,CD,CHIN,CONT,D    P500 110
      COMMON DA,DP,DISP,EDGE,EV,FORM,FS,ID,ITILT,KD,LATN,LTNC,NATOM,NCD P500 120
      COMMON NJ,NJ2,NOUT,NSD,NSYM,ORGN,P,PA,PAC,PAT,Q,RTPV,RES,RMS,SCAL1P500 130
      COMMON SCAL2,SCL,STHD,TAPED,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2    P500 140
      COMMON V3,V4,V5,V6,UNIV,XLNG,XO,XT                                 P500 150
      NG=0                                                               P500 160
      IF(NJ2-11)500,700,710                                              P500 170
  500 IF(NJ2-1)710,501,510                                               P500 180
  501 T1=AIN(1)                                                          P500 190
      CALL ATOM(T1,ORGN)                                                 P500 200
      IF(NG)502,504,502                                                  P500 210
  502 CALL ERPRT(T1,501)                                                 P500 220
      CALL EXIT                                                          P500 230
  504 DO 506 K=1,4                                                       P500 240
      T1=AIN(K+1)                                                        P500 250
      CALL ATOM(T1,V(1,K))                                               P500 260
      IF(NG)502,506,502                                                  P500 270
  506 CONTINUE                                                           P500 280
      DO 507 J=1,3                                                       P500 290
      V1(J)=V(J,2)-V(J,1)                                                P500 300
  507 V2(J)=V(J,4)-V(J,3)                                                P500 310
      INDX=1                                                             P500 320
      IF(AIN(7))508,509,508                                              P500 330
  508 INDX=2                                                             P500 340
  509 CALL AXES(V1,V2,RTPV,INDX)                                         P500 350
      GO TO 675                                                          P500 360
  510 IF(NJ2-4)515,511,599                                               P500 370
C     ***** SHIFT ORIGIN FOR PROJECTION AXIS (IN INCHES) *****           P500 380
  511 DO 513 J=1,3                                                       P500 390
      DO 512 K=1,3                                                       P500 400
  512 ORGN(J)=ORGN(J)+RTPV(J,K)*AIN(K)/SCAL1                             P500 410
  513 XO(J)=XO(J)+AIN(J)                                                 P500 420
      GO TO 675                                                          P500 430
C     ***** FORM ROTATION MATRIX *****                                   P500 440
  515 DO 552 L=1,130,2                                                   P500 450
      I=AIN(L)                                                           P500 460
      IF(I) 552,552,516                                                  P500 470
  516 Z=AIN(L+1)*1.7453293E-2                                            P500 480
      T1=COS(Z)                                                          P500 490
      T2=SIN(Z)                                                          P500 500
      I3=MOD(I+2,3)+1                                                    P500 510
      I1=MOD(I3,3)+1                                                     P500 520
      I2=MOD(I1,3)+1                                                     P500 530
      RR(I1,I1)=T1                                                       P500 540
      RR(I1,I2)=T2                                                       P500 550
      RR(I1,I3)=0.0                                                      P500 560
      RR(I2,I1)=-T2                                                      P500 570
      RR(I2,I2)=T1                                                       P500 580
      RR(I2,I3)=0.0                                                      P500 590
      RR(I3,I1)=0.0                                                      P500 600
      RR(I3,I2)=0.0                                                      P500 610
      RR(I3,I3)=1.0                                                      P500 620
      CALL MM(RTPV,RR,V)                                                 P500 630
      IF(NJ2-3)518,525,599                                               P500 640
  518 DO 522 J=1,3                                                       P500 650
      DO 522 I=1,3                                                       P500 660
  522 RTPV(I,J)=V(I,J)                                                   P500 670
      GO TO 552                                                          P500 680
  525 DO 520 J=1,3                                                       P500 690
      DO 520 I=1,3                                                       P500 700
  520 UNIV(I,J)=V(I,J)                                                   P500 710
      GO TO 552                                                          P500 720
  532 IF(NJ2-3)535,552,599                                               P500 730
  535 I=MOD(-I,3)                                                        P500 740
      DO 542 J=1,I                                                       P500 750
      DO 542 K=1,3                                                       P500 760
      T1=RTPV(K,3)                                                       P500 770
      RTPV(K,3)=RTPV(K,2)                                                P500 780
      RTPV(K,2)=RTPV(K,1)                                                P500 790
  542 RTPV(K,1)=T1                                                       P500 800
  552 CONTINUE                                                           P500 810
      IF(NJ2-3)670,582,599                                               P500 820
  582 CALL MM(AA,UNIV,AAUBH)                                             P500 830
      GO TO 699                                                          P500 840
  599 IF(NJ2-5)699,600,607                                               P500 850
  600 IF(LATN-1)605,610,610                                              P500 860
  605 NG=12                                                              P500 870
  606 CALL ERPRT(0.,506)                                                 P500 880
      CALL EXIT                                                          P500 890
  607 IF(NJ2-8)699,608,710                                               P500 900
  608 IF(LATN-3)605,610,610                                              P500 910
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  610 DO 612 J=1,3                                                      P500 920
      V2(J)=0.0                                                         P500 930
      DO 612 I=1,3                                                      P500 940
  612 D9(I,J)=0.0                                                       P500 950
      AWT=0.0                                                           P500 960
      DO 620 K=1,LATM                                                   P500 970
      CALL ATOM(ATOMS(1,K),ATOMS(2,K))                                  P500 980
      T2=1.0                                                            P500 990
      IF(NCD)618,618,613                                                P5001000
  613 T1=ATOMS(1,K)/100000.                                             P5001010
      DO 616 J=1,NCD                                                    P5001020
      T2=CD(1,J)                                                        P5001030
      IF(T1-ND(1,J))616,614,614                                         P5001040
  614 IF(ND(2,J)-T1)616,618,618                                         P5001050
  616 CONTINUE                                                          P5001060
      GO TO 620                                                         P5001070
  618 AWT=AWT+T2                                                        P5001080
      DO 619 J=1,3                                                      P5001090
  619 V2(J)=V2(J)+ATOMS(J+1,K)*T2                                       P5001100
  620 CONTINUE                                                          P5001110
      IF(AWT)605,605,621                                                P5001120
C     ***** PUT ORIGIN AT CENTER OF GRAVITY *****                       P5001130
  621 DO 622 J=1,3                                                      P5001140
  622 ORGN(J)=V2(J)/AWT                                                 P5001150
      IF(NJ2-6)630,624,710                                              P5001160
C     ***** FORM PRODUCT-MOMENT MATRIX FOR ATOMS IN ATOM LIST *****     P5001170
  624 DO 630 K=1,LATM                                                   P5001180
      T2=1.0                                                            P5001190
      IF(NCD)628,628,625                                                P5001200
  625 T1=ATOMS(1,K)/100000.                                             P5001210
      DO 627 J=1,NCD                                                    P5001220
      T2=CD(1,J)                                                        P5001230
      IF(T1-ND(1,J))627,626,626                                         P5001240
  626 IF(ND(2,J)-T1)627,628,628                                         P5001250
  627 CONTINUE                                                          P5001260
      GO TO 630                                                         P5001270
  628 DO 629 J=1,3                                                      P5001280
      T1=(ATOMS(J+1,K)-ORGN(J))*T2                                      P5001290
      DO 629 I=1,3                                                      P5001300
  629 D9(I,J)=T1*(ATOMS(I+1,K)-ORGN(I))+D9(I,J)                         P5001310
      T1=0.01/(D9(1,1)+D9(2,2)+D9(3,3))                                 P5001320
  630 CONTINUE                                                          P5001330
      DO 632 J=1,3                                                      P5001340
      DO 632 I=1,3                                                      P5001350
  632 D9(I,J)=D9(I,J)*T1                                                P5001360
C     ***** TRANSFORM TO INERTIAL AXIS SYSTEM *****                     P5001370
      CALL MM(D9,AA,DA)                                                 P5001380
      CALL EIGEN(DA,DNS,PAT)                                            P5001390
      IF(DNS(2))605,605,635                                             P5001400
  635 IF(NG)643,633,646                                                 P5001410
C     ***** MAKE SURE VECTORS ARE ORTHOGONAL --> NEW REFERENCE VECTORS *P5001420
  633 CALL AXES(PAT(1,3),PAT(1,1),REFV,-1)                              P5001430
      GO TO 665                                                         P5001440
C     ***** TWO EQUAL EIGENVECTORS SPECIAL CASE *****                   P5001450
  640 IF(NJ2-4)645,665,665                                              P5001460
  645 N=NJ2-3                                                           P5001470
      CALL UNIT(PAT(1,N),V1,-1)                                         P5001480
      DO 650 K=1,3                                                      P5001490
      IF(ABS(VMV(V1,AA,REFV(1,K)))-.50)655,650,650                      P5001500
  650 CONTINUE                                                          P5001510
  655 CALL AXES(V1,REFV(1,K),DA,-1)                                     P5001520
      DO 660 K=1,3                                                      P5001530
      L=MOD(N-K+2,3)+1                                                  P5001540
      DO 660 J=1,3                                                      P5001550
  660 REFV(J,L)=DA(J,K)                                                 P5001560
  665 NG=0                                                              P5001570
  670 CALL MM(AA,REFV,AAREV)                                            P5001580
  675 DO 690 J=1,3                                                      P5001590
      DO 690 I=1,3                                                      P5001600
      WRKV(I,J)=REFV(I,J)                                               P5001610
  690 AAWRK(I,J)=AAREV(I,J)                                             P5001620
C     ***** ELIMINATE ALL PREVIOUSLY STORED OVERLAP INFORMATION ****    P5001630
C       *** (ALL INSTRUCTIONS FROM 501 THROUGH 510 DO THIS) *****       P5001640
  695 CALL LAP500(0)                                                    P5001650
      GO TO 710                                                         P5001660
C     ***** STORE NEW OVERLAP INFORMATION (INSTRUCTION 511) *****       P5001670
  700 CALL LAP500(1)                                                    P5001680
  710 RETURN                                                            P5001690
      END                                                               P5001700
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      SUBROUTINE P600                                                   P600  10
C     ***** SCALING AND CENTERING FUNCTIONS *****                       P600  20
      DIMENSION MAX(3),SCAL(8),X(3),XMAX(3),XMIN(3),Z(2)                P600  30
      REAL*8 CHEM                                                       P600  40
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    P600  50
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(144),CONT(5),D(3,110)P600  60
      DIMENSION DA(3,3),DP(2,120),EV(3,144),FS(3,3,48),ND(5,10),ORGN(3) P600  70
      DIMENSION P(3,144),PA(3,3,144),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) P600  80
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,48)   P600  90
      DIMENSION V7(3,8),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   P600 100
      DIMENSION XLNG(3),XO(3),XT(3)                                     P600 110
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   P600 120
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTMO,NATOM,NCD P600 130
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL P600 140
      COMMON SCAL2,SCL,SYMB,TAPEO,THETA,TITLE,TITLE2,TS,VIEW,V7,V1,V2   P600 150
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                P600 160
C     ***** DEL = 1. FOR INCREMENTAL FUNCTIONS *****                    P600 170
C     ***** DEL = 0. FOR REGULAR FUNCTIONS *****                        P600 180
      DEL=FLOAT(MOD(NJ2/10,2))                                          P600 190
      NJ2=MOD(NJ2,10)                                                   P600 200
C     ***** EXPLICIT ORIGIN AND SCALE *****                             P600 210
      IF(AIN(1))602,604,602                                             P600 220
  602 XO(1)=AIN(1)+XO(1)*DEL                                            P600 230
  604 IF(AIN(2))606,608,606                                             P600 240
  606 XO(2)=AIN(2)+XO(2)*DEL                                            P600 250
  608 IF(AIN(3))612,612,609                                             P600 260
  609 IF(DEL)611,611,610                                                P600 270
  610 SCAL1=SCAL1*AIN(3)                                                P600 280
      GO TO 612                                                         P600 290
  611 SCAL1=AIN(3)                                                      P600 300
  612 IF(AIN(4))616,616,614                                             P600 310
C     ***** SET ELLIPSOID SCALE FACTOR *****                            P600 320
  614 SCAL2=AIN(4)                                                      P600 330
C     ***** AUTOMATIC ORIGIN AND/OR SCALE *****                         P600 340
  616 IF(NJ2-2)790,622,620                                              P600 350
  620 XO(1)=XLNG(1)*.5                                                  P600 360
      XO(2)=XLNG(2)*.5                                                  P600 370
  622 IF(NJ2-3)625,640,625                                              P600 380
  625 SCAL1=1.                                                          P600 390
  630 IF(LATM-1)635,635,640                                             P600 400
  635 NG=12                                                             P600 410
      CALL ERPNT(0.,602)                                                P600 420
      CALL EXIT                                                         P600 430
  640 DO 650 J=1,3                                                      P600 440
      XMAX(J)=-1.E5                                                     P600 450
  650 XMIN(J)=1.E5                                                      P600 460
C     ***** FIT BOX AROUND SET OF ATOMS *****                           P600 470
      DO 670 I=1,LATM                                                   P600 480
      CALL XYZ(ATOMS(1,I),ATOMS(2,I),3)                                 P600 490
      IF(NG)652,653,652                                                 P600 500
  652 CALL ERPNT(ATOMS(1,I),600)                                        P600 510
      GO TO 670                                                         P600 520
  653 DO 668 J=1,3                                                      P600 530
      T1=ATOMS(J+1,I)                                                   P600 540
      IF(XMAX(J)-T1)655,660,660                                         P600 550
  655 XMAX(J)=T1                                                        P600 560
      MAX(J)=I                                                          P600 570
  660 IF(T1-XMIN(J))665,668,668                                         P600 580
  665 XMIN(J)=T1                                                        P600 590
  668 CONTINUE                                                          P600 600
  670 CONTINUE                                                          P600 610
C     ***** ANCHOR ATOM *****                                           P600 620
      K=MAX(3)                                                          P600 630
      SMULT=1.                                                          P600 640
      DO 700 N=1,5                                                      P600 650
      IF(N-2)700,675,670                                                P600 660
C     ***** CHECK VIEW DISTANCE *****                                   P600 670
  675 IF(VIEW)705,705,680                                               P600 680
  678 IF(NJ2-3)680,705,680                                              P600 690
  680 T1=ATOMS(4,KK)*SMULT                                              P600 700
      IF(VIEW-5.*T1)685,690,690                                         P600 710
C     ***** INCREASE VIEW DISTANCE *****                                P600 720
  685 VIEW=2.*T1                                                        P600 730
C     ***** FIND PERSPECTIVE PROJECTION LIMITS *****                    P600 740
  690 DO 700 J=1,2                                                      P600 750
      XMAX(J)=-1.E5                                                     P600 760
  700 XMIN(J)=1.E5                                                      P600 770
      DO 72  I=1,LATM                                                   P600 780
      DO 70  J=1,3                                                      P600 790
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  705 X(J)=ATOMS(J+1,I)*SMULT
      T2=VIEW/(VIEW-X(3))
      DO 725 J=1,2
      T1=X(J)*T2
      IF(XMAX(J)-T1)710,715,715
  710 XMAX(J)=T1
  715 IF(T1-XMIN(J))720,725,725
  720 XMIN(J)=T1
  725 CONTINUE
C     ***** DEFINE PARAMETERS *****
  740 IF(NJ2 - 3) 745,742,755
  742 SMUL3=1.
      GO TO 765
C     ***** AUTOMATIC SCALE ONLY *****
  745 DO 750 J=1,2
      T2=XO(J)
      SCAL(J)=(BORD-T2)/XMIN(J)
  750 SCAL(J+2)=(XLNG(J)-BORD-T2)/XMAX(J)
      SMUL2=AMIN1(SCAL(1),SCAL(2),SCAL(3),SCAL(4))
      GO TO 780
C     ***** AUTOMATIC SCALE AND POSITION *****
  755 DO 760 J=1,2
  760 SCAL(J)=(XLNG(J)-BORD*2.)/(XMAX(J)-XMIN(J))
      SMUL2=AMIN1(SCAL(1),SCAL(2))
C     ***** AUTOMATIC POSITION *****
  765 DO 770 J=1,2
  770 XO(J)=.5*(XLNG(J)-SMUL2*(XMAX(J)+XMIN(J)))
  780 SMULT=SMULT*SMUL2
      VIEW=VIEW*SMUL2
  785 SCAL1=SCAL1*SMULT
  790 SCL=SCAL1*SCAL2
C     ***** ELIMINATE ALL PREVIOUSLY STORED OVERLAP INFORMATION *****
      CALL LAP900(0)
      RETURN
      END


      SUBROUTINE P700
C     ***** SUBROUTINE TO DRAW ELLIPSOIDS *****
      DIMENSION EYE(3),VIEWV(3),X(3),Z(3)
      REAL*8 CHEM
      DIMENSION A(9),AA(3,3),AARDV(3,3),AAWRK(3,3),AID(3,3),AIN(140)
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(166),CONT(5),D(3,11)
      DIMENSION DA(3,3),DP(2,120),EV(3,166),FS(3,3,96),NG(5,10),ORGN(3)
      DIMENSION P(3,166),PA(3,3,166),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3)
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,96)
      DIMENSION VT(3,4),V1(6),V2(3),V3(3),V4(3),V5(3),V6(3),WRK(3,3)
      DIMENSION XLNG(3),XO(3),XT(3)
      COMMON NG,A,AA,AARDV,AAWRK,AID,AIN,ATOMS,BB,BORD,CD,CHEM,CONT,D
      COMMON DA,DP,DISP,EDGE,EV,FORM,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1
      COMMON SCAL2,SCL,SYMB,TAPED,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT
C     ***** SET ELLIPSOID GRAPHIC DETAILS *****
      ITILT=0
      NG=0
      NFIRST=1
      NPLANE=AIN(1)
      IF(NPLANE-4)720,715,720
  715 NFIRST=4
      NPLANE=4
  720 NSOLID=AIN(2)
      NCURV=64/2**( IABS(NSOLID))
      LINES=AIN(3)
      NDASH=AIN(4)
      CHSYM=AIN(5)
      DH=AIN(6)-CHSYM*17./7.
      DV=AIN(7)-CHSYM*.5
C     ***** ESTABLISH REFERENCE POINT OF VIEW *****
      T1=1.E6
      IF(VIEW) 740,740,735
  735 T1=VIEW/SCAL1
  740 DO 741 J=1,3
  741 EYE(J)=REFV(J,3)*T1+ORGN(J)
      LAST=-1
C     ***** LOOP THROUGH ATOM LIST *****
      DO 1105 ITOM=1,LATM
      T1=ATOMS(1,ITOM)
      IF(AIN(10))744,744,742
  742 T2=AINT(T1/100000.)
      IF(T2-AIN(10)) 1105,743,743
  743 IF(AIN(11)-T2) 1105,744,744
  744 CALL XYZ(T1,X,3)
      IF(NG) 750,746,750
  746 CALL PLTXY(X,Z)
      K=T1/100000.
      L=T1-FLOAT (K)*100000.
      IF(NJ2-10) 747,750,750
  747 LNS=MOD(LNS+1,18)
      IF(LNS) 749,748,749
  748 WRITE (NOUT,751) (TITLE(I),I=1,18)
      WRITE (NOUT,752)
  749 WRITE (NOUT,750)CHEM(K),K,L,Z(1),Z(2),(X(I),I=1,3),(XT(
     1I),I=1,3)
  750 FORMAT(1H 10X,A6,1H (I1,I5,1H)  2F8.3,1X,3F8.3,11X,3F8.3)
  751 FORMAT(1H110X,18A4)
  752 FORMAT(1H0,10X,10HSYMBOL    ATOM CODE13,16HPLOTTER X,Y (IN.) 3X,21HCR
     1YSTAL X,Y,Z (IN.)15X,30HCRYSTAL SYSTEM X,Y,Z/1H 10X,65H(DIRECTIO
     2N COSINES(I,J),I=1,3),REFV(J),J=1,3)13X,62HFOR PRINCIPAL AXES BASE
     3D ON WORKING SYSTEM/1H )
  754 IF(RMAP-BORD*.75)755,760,760
  755 NG=15
  758 CALL ERPNT(T1,700)
      GO TO 1105
C     ***** CALL OVERLAP ROUTINE *****
  760 ICO=0
      CALL LAP700(ITOM,ICO)
      IF(ICO) 762,764,764
C     ***** OMIT HIDDEN ATOM *****
  762 NG=14
      GO TO 758
  764 IF(CHSYM) 775,775,765
C     ***** PLOT CHEMICAL SYMBOLS *****
  765 T4=1.
      IF(VIEW) 767,767,766
  766 T4=VIEW/(VIEW-X(3))
  767 T3=CHSYM*T4
      T4=DISP*T4*0.5
      V1(1)=Z(1)+DH*SYMB(1,1)+DV*SYMB(1,2)
      V1(2)=Z(2)+DH*SYMB(2,1)+DV*SYMB(2,2)
      V1(3)=Z(3)
      CALL PLTXY(V1,V3)
      IF(EDGE-CHSYM) 775,768,768
  768 V2(3)=0.
      DO 770 I=1,3,2
      V2(1)=V3(1)+FLOAT(I-2)*T4
      DO 770 J=1,3,2
      V2(2)=V3(2)+FLOAT(J-2)*T4
      CALL SYMBOL(V2(1),V2(2),T3,CHEM(K),THETA,6)
      IF(T4) 775,775,770
  770 CONTINUE
  775 IF(NPLANE) 1105,1105,780
C     ***** ELLIPSOID PRINC VECTORS TOWARD VIEWER *****
  780 CALL PAXES(T1,2)
      IF(NG) 758,783,758
  783 CALL DIFV(EYE,XT,VIEWV)
      CALL UNIT(VIEWV,VIEWV,-1)
      CALL VM(VIEWV,AA,V2)
      DO 795 I=1,3
      IF(VV(V2,PAT(1,I)))785,795,795
  785 DO 790 J=1,3
      PAC(J,I)=-PAC(J,I)
  790 PAT(J,I)=-PAT(J,I)
  795 CONTINUE
      DO 800 J=1,3
      PAC(J,4)=PAC(J,1)
  800 PAC(J,5)=PAC(J,2)
      IF(NJ2-10) 802,803,803
  801 FORMAT(1H 13X,3(3X,3F8.4,F8.3)/1H )
  802 WRITE (NOUT,801) ((PAC(J,K),J=1,3),RMS(K) ,K=1,3)
C     ***** V6 = VECTOR NORMAL TO POLAR PLANE *****
  803 CALL VM(VIEWV,AAWRK,V6)
      CALL UNIT(V6,V6,1)
      CALL MV(Q,V6,V4)
      CALL UNIT(V4,V4,1)
C     ***** SET PLOTTING RESOLUTION FOR ELLIPSOID *****
      T3=RMS(3)*SCL
      NRESOL=1
      NDIS=5
      DO 805 J=1,3
      IF(T3-RES(J)) 804,810,810
  804 NDIS=NDIS-1
  805 NRESOL=NRESOL*2
  810 NRES1=NRESOL+1
C     ***** LOOP THROUGH PRINC AND POLAR PLANES *****
      DO 1100 II=NFIRST,NPLANE
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      II0=MOD(II+2,3)+1                                                 P7001300
      II1=MOD(II,3)+1                                                   P7001310
      II2=MOD(II+1,3)+1                                                 P7001320
C     ***** GENERATE CONJUGATE DIAMETERS *****                          P7001330
      IF(.99999- ABS(VV(V4,PAC(1,II2))))820,820,830                     P7001340
  820 T1=RMS(II0)*SCL                                                   P7001350
      T2=RMS(II1)*SCL                                                   P7001360
      DO 825 J=1,3                                                      P7001370
      DA(J,1)=PAC(J,II0)*T1                                             P7001380
  825 DA(J,2)=PAC(J,II1)*T2                                             P7001390
      GO TO 850                                                         P7001400
  830 CALL NORM(PAC(1,II0),PAC(1,II1),V1,1)                             P7001410
      CALL NORM(V1,V4,V2,1)                                             P7001420
      CALL UNITY(V2,V2,1)                                               P7001430
      CALL MV(Q,V2,V3)                                                  P7001440
      IF(II-4) 835,840,840                                              P7001450
  835 CALL NORM(V3,V1,V5,1)                                             P7001460
      GO TO 843                                                         P7001470
  840 CALL NORM(V3,V4,V5,1)                                             P7001480
  843 CALL UNITY(V5,V5,1)                                               P7001490
      T1=SCL/SQRT(VMV(V2,Q,V2))                                         P7001500
      T2=SCL/SQRT(VMV(V5,Q,V5))                                         P7001510
      DO 845 J=1,3                                                      P7001520
      DA(J,1)=V2(J)*T1                                                  P7001530
  845 DA(J,2)=V5(J)*T2                                                  P7001540
C     ***** INTEGRATE ELLIPSE *****                                     P7001550
  850 CALL RADIAL(NDIS)                                                 P7001560
      IF(II-4) 900,851,851                                              P7001570
  851 IF(NSOLID) 859,859,852                                            P7001580
C     ***** PLOT DOTTED BOUNDARY ELLIPSE *****                          P7001590
  852 IF(NDOT-NRESOL) 853,855,855                                       P7001600
  853 CALL RADIAL(NSOLID-1)                                             P7001610
  855 CALL PROJ(D,DP,X,XO,VIEW,1,129,NDOT)                              P7001620
      DO 857 J=1,129,NDOT                                               P7001630
      CALL DRAW(DP(1,J),DISP,DISP,3)                                    P7001640
      DO 856 I=1,3,2                                                    P7001650
      T1=FLOAT(I-2)*DISP                                                P7001660
      DO 856 K=1,3,2                                                    P7001670
      T2=FLOAT(K-2)*DISP                                                P7001680
      CALL DRAW(DP(1,J),T1,T2,2)                                        P7001690
      IF(DISP) 857,857,856                                              P7001700
  856 CONTINUE                                                          P7001710
  857 CONTINUE                                                          P7001720
      GO TO 1100                                                        P7001730
C     ***** PLOT SOLID BOUNDARY ELLIPSE *****                           P7001740
  859 CALL PROJ(E,DP,X,XO,VIEW,1,129,NRESOL)                            P7001750
      CALL DRAW(DP,0.,0.,3)                                             P7001760
      DO 860 J=NRES1,129,NRESOL                                         P7001770
  860 CALL DRAW(DP(1,J),0.,0.,2)                                        P7001780
      IF(DISP) 1100,1100,865                                            P7001790
C     ***** BOUNDARY ANNULUS AS A LINEAR FUNCTION OF HEIGHT *****       P7001800
  865 CALL DIFV(XT,ORGN,V1)                                             P7001810
      T5=VV(V1,AAREV(1,3))*SCAL1                                        P7001820
      NCYCLE=.5+(AIN(8)+T5*AIN(9))/DISP                                 P7001830
      IF(NCYCLE) 1100,1100,870                                          P7001840
  870 T3=(2.*DISP)/(T1+T2)                                              P7001850
C     ***** INCREASE ANNULAR THICKNESS *****                            P7001860
      DO 875 I=1,NCYCLE                                                 P7001870
      T4=1.+T3*FLOAT(I)                                                 P7001880
      DO 875 J=1,129,NRESOL                                             P7001890
  875 CALL DRAW(DP(1,J),D(1,J)*T4,D(2,J)*T4,2)                          P7001900
      GO TO 1100                                                        P7001910
  900 CALL PROJ(D,DP,X,XO,VIEW,1,65,NRESOL)                             P7001920
C     ***** PLOT HALF AN ELLIPSE *****                                  P7001930
      CALL DRAW(DP,0.,0.,3)                                             P7001940
      DO 905 J=NRES1,65,NRESOL                                          P7001950
  905 CALL DRAW(DP(1,J),0.,0.,2)                                        P7001960
      IF(DISP) 930,930,910                                              P7001970
C     ***** ACCENTUATE FRONT HALF *****                                 P7001980
  910 DO 925 I=1,3,2                                                    P7001990
      T2=FLOAT(I-2)*DISP                                                P7002000
      DO 915 J=1,65,NRESOL                                              P7002010
      K=66-J                                                            P7002020
  915 CALL DRAW(DP(1,K),DISP,T2,2)                                      P7002030
      DO 925 K=1,65,NRESOL                                              P7002040
  925 CALL DRAW(DP(1,K),-DISP,-T2,2)                                    P7002050
  930 IF(NSOLID) 940,967,935                                            P7002060
  935 L=NDOT                                                            P7002070
      IF(NDOT-NRESOL) 936,945,940                                       P7002080
  936 CALL RADIAL(NSOLID-1)                                             P7002090
      GO TO 945                                                         P7002100
  940 L=NRESOL                                                          P7002110
  945 CALL PROJ(D(1,65),DP(1,65),X,XO,VIEW,1,65,L)                      P7002120
      IF(NSOLID) 960,967,950                                            P7002130
C     ***** DOTTED LINE ON REVERSE SIDE *****                           P7002140
  950 DO 958 J=65,129,NDOT                                              P7002150
      CALL DRAW(DP(1,J),DISP,DISP,3)                                    P7002160
      DO 955 I=1,3,2                                                    P7002170
      T1=FLOAT(I-2)*DISP                                                P7002180
      DO 955 K=1,3,2                                                    P7002190
      T2=FLOAT(K-2)*DISP                                                P7002200
      CALL DRAW(DP(1,J),T1,T2,2)                                        P7002210
      IF(DISP) 958,958,955                                              P7002220
  955 CONTINUE                                                          P7002230
  958 CONTINUE                                                          P7002240
      GO TO 967                                                         P7002250
C     ***** SINGLE LINE ON REVERSE SIDE *****                           P7002260
  960 DO 965 J=65,129,NRESOL                                            P7002270
  965 CALL DRAW(DP(1,J),0.,0.,2)                                        P7002280
C     ***** DETAIL INTERIOR FEATURES *****                              P7002290
  967 T2=NDASH*2                                                        P7002300
      DO 975 J=1,3                                                      P7002310
      T1=PAC(J,II0)*RMS(II0)*SCL                                        P7002320
      DA(J,1)=T1                                                        P7002330
      DA(J,2)=PAC(J,II1)*RMS(II1)*SCL                                   P7002340
      DA(J,3)=0.                                                        P7002350
      IF(NDASH) 975,975,970                                             P7002360
  970 V1(J)=-T1                                                         P7002370
      V2(J)=T1/T2                                                       P7002380
  975 CONTINUE                                                          P7002390
      IF(NDASH) 987,987,980                                             P7002400
C     ***** DASHED LINE FOR REVERSE AXIS *****                          P7002410
  980 DO 985 J=1,NDASH                                                  P7002420
      DO 985 K=1,2                                                      P7002430
      L=4-K                                                             P7002440
      CALL PROJ(V1,DP,X,XO,VIEW,1,1,1)                                  P7002450
      CALL DRAW(DP,0.,0.,L)                                             P7002460
      DO 985 I=1,3                                                      P7002470
  985 V1(I)=V1(I)+V2(I)                                                 P7002480
C     ***** SOLID LINE FOR FORWARD AXIS *****                           P7002490
  987 IF(LINES) 1100,1100,988                                           P7002500
  988 CALL PROJ(DA,DP,X,XO,VIEW,1,3,1)                                  P7002510
      T1=DISP*.5                                                        P7002520
      DO 990 I=1,3,2                                                    P7002530
      T2=FLOAT(I-2)*T1                                                  P7002540
      CALL DRAW(DP,T1,T2,3)                                             P7002550
      CALL DRAW(DP(1,3),T1,T2,2)                                        P7002560
      IF(DISP) 1000,1000,989                                            P7002570
  989 CALL DRAW(DP(1,3),-T1,T2,2)                                       P7002580
  990 CALL DRAW(DP,-T1,T2,2)                                            P7002590
C     ***** SHADE QUADRANT BETWEEN TWO PRINCIPAL AXES *****             P7002600
 1000 L=LINES-1                                                         P7002610
      IF(L) 1100,1100,1005                                              P7002620
 1005 T2=LINES                                                          P7002630
      DO 1025 I=1,L                                                     P7002640
      T1=FLOAT(I)/T2                                                    P7002650
      T3=SQRT(1.-T1*T1)                                                 P7002660
      IF(MOD(I,2)) 1010,1015,1010                                       P7002670
 1010 M=I*2                                                             P7002680
      N=M-1                                                             P7002690
      GO TO 1020                                                        P7002700
 1015 N=I*2                                                             P7002710
      M=N-1                                                             P7002720
 1020 DO 1025 J=1,3                                                     P7002730
      T4=DA(J,1)*T1                                                     P7002740
      D(J,M)=T4                                                         P7002750
 1025 D(J,N)=DA(J,2)*T3+T4                                              P7002760
      L=L*2                                                             P7002770
      CALL PROJ(D,DP,X,XO,VIEW,1,L,1)                                   P7002780
      DO 1030 I=2,L,2                                                   P7002790
      CALL DRAW(DP(1,I-1),0.,0.,3)                                      P7002800
 1030 CALL DRAW(DP(1,I),0.,0.,2)                                        P7002810
 1100 CONTINUE                                                          P7002820
 1105 CONTINUE                                                          P7002830
C     ***** ELIMINATE LOCAL OVERLAP INFORMATION BEFORE RETURNING *****  P7002840
      CALL LAP500(-1)                                                   P7002850
      RETURN                                                            P7002860
      END                                                               P7002870


      SUBROUTINE P800                                                   P800  10
C     ***** SUBROUTINE FINDS ATOM PAIRS FOR BONDS *****                 P800  20
      DIMENSION TA(3),M1(6)                                             P800  30
      REAL*8 CHEM                                                       P800  40
      DIMENSION A(3),AA(3,3),AAREV(3,3),AAWRK(3,3),ATN(3,3),AIN(140)    P800  50
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(166),CONT(5),D(3,130)P800  60
      DIMENSION DA(3,3),DP(2,130),EV(3,166),FS(3,3,96),KD(5,10),NCAN(3) P800  70
      DIMENSION P(3,166),PA(3,3,166),PAC(3,4),PAT(3,3),Q(3,3),REFV(3,3) P800  80
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      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,48)   F800  90
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   F800 100
      DIMENSION XLNG(3),XO(3),XT(3)                                     F800 110
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BBOX,CD,CHEM,CONT,D   F800 120
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LINO,NATOM,NCD F800 130
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1F800 140
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   F800 150
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                F800 160
      LNS=0                                                             F800 170
      IF(MOD(NJ2,10)-2)805,848,848                                      F800 180
C     ***** EXPLICIT DESCRIPTION *****                                  F800 190
  805 II=0                                                              F800 200
      IF(NCD)810,810,815                                                F800 210
  810 NG=11                                                             F800 220
      CALL ERPNT(0.,NJ*100+NJ2)                                         F800 230
      GO TO 980                                                         F800 240
  815 II=II+1                                                           F800 250
      IF(IN-II)980,980,820                                              F800 260
  820 T1=AIN(II)                                                        F800 270
      IF(T1)815,815,825                                                 F800 280
  825 II=II+1                                                           F800 290
      T2=AIN(II)                                                        F800 300
      IF(T2)815,815,830                                                 F800 310
  830 IF(NJ2-10)832,838,838                                             F800 320
  832 LNS=MOD(LNS+4,56)                                                 F800 330
      IF(LNS)834,834,838                                                F800 340
  834 WRITE (NOUT,835) (TITLE(I),I=1,18)                                F800 350
  835 FORMAT(1H1,10X,18A4)                                              F800 360
      WRITE (NOUT,837)                                                  F800 370
  837 FORMAT(1H0 10X,10HSYMBOL    ATOM CODE11X,16HPLOTTER X,Y (IN.) 6X,21HCAF800 380
     1RTESIAN X,Y,Z (IN.) 17X,27HCRYSTAL SYSTEM X,Y,Z/1H )              F800 390
C     ***** CHECK IF BOND ATOMS ARE IN ATOMS LIST (FOR OVERLAP CALC) ***F800 400
  838 NA1=0                                                             F800 410
      NA2=0                                                             F800 420
      IF(LATM-2)845,839,839                                             F800 430
  839 N2=2                                                              F800 440
      DO 844 N=1,LATM                                                   F800 450
      T3=ATOMS(1,N)                                                     F800 460
      IF(T3-T1)841,840,841                                              F800 470
  840 NA1=N                                                             F800 480
      GO TO 843                                                         F800 490
  841 IF(T3-T2)844,842,844                                              F800 500
  842 NA2=N                                                             F800 510
  843 N2=N2-1                                                           F800 520
      IF(N2)845,845,844                                                 F800 530
  844 CONTINUE                                                          F800 540
  845 IF(NA2-NA1)846,847,847                                            F800 550
  846 NA3=NA1                                                           F800 560
      NA1=NA2                                                           F800 570
      NA2=NA3                                                           F800 580
      T3=T1                                                             F800 590
      T1=T2                                                             F800 600
      T2=T3                                                             F800 610
  847 CALL BOND(T1,T2,1,NA1,NA2)                                        F800 620
      GO TO 815                                                         F800 630
C     ***** IMPLICIT DESCRIPTION *****                                  F800 640
  848 IF(LATM-2)980,850,850                                             F800 650
  850 SCAL3=SCAL1                                                       F800 660
      SCAL1=1.                                                          F800 670
      DO 855 I=1,LATM                                                   F800 680
  855 CALL XYZ(ATOMS(1,I),ATOMS(2,I),2)                                 F800 690
      SCAL1=SCAL3                                                       F800 700
      IF(NCD)810,810,860                                                F800 710
  860 WRITE (NOUT,861)                                                  F800 720
  861 FORMAT(1H0 10X,20HBOND SELECTION CODES//11X,94H(SEQUENCE(S)) (SEQUENF800 730
     1CE(S)) (BOND) (DISTANCES) ( BOND ) (PERSP.--LABELS) (NORMAL--LABELS) (F800 740
     2DIGITS) /11X,93H( MIN MAX )( MIN MAX ) (TYPE) (MIN   MAX) (RADIF800 750
     3US) (HEIGHT  OFFSET) (HEIGHT  OFFSET) (NUMBER))                   F800 760
      DMAX=0.                                                           F800 770
      DO 870 I=1,NCD                                                    F800 780
      IF(DMAX-CD(2,I))865,870,870                                       F800 790
  865 DMAX=CD(2,I)                                                      F800 800
  870 WRITE (NOUT,871) (KD(J,I),J=1,5),(CD(J,I),J=1,8)                  F800 810
  871 FORMAT(1H 10XI6,I5,I8,I5,I8,2F6.2,5F8.3,F7.0)                     F800 820
      DMAX=DMAX*DMAX                                                    F800 830
C     ***** LOOP THROUGH ATOMS ARRAY *****                              F800 840
      DO 977 N=1,LATM                                                   F800 850
      NA1=N                                                             F800 860
      T1=ATOMS(1,N)                                                     F800 870
      IA(1)=T1/100000.                                                  F800 880
      IA(3)=IA(1)                                                       F800 890
      U1(1)=ATOMS(2,N)                                                  F800 900
      U1(2)=ATOMS(3,N)                                                  F800 910
      U1(3)=ATOMS(4,N)                                                  F800 920
      L=N+1                                                             F800 930
      IF(LATM-L)977,872,872                                             F800 940
  872 DO 975 M=L,LATM                                                   F800 950
      NA2=M                                                             F800 960
      DIST=(ATOMS(2,M)-U1(1))**2                                        F800 970
      IF(DMAX-DIST)975,873,873                                          F800 980
  873 DIST=DIST+(ATOMS(3,M)-U1(2))**2                                   F800 990
      IF(DMAX-DIST)975,874,874                                          F8001000
  874 DIST=DIST+(ATOMS(4,M)-U1(3))**2                                   F8001010
      IF(DMAX-DIST)975,875,875                                          F8001020
  875 DIST=SQRT(DIST)                                                   F8001030
      T2=ATOMS(1,M)                                                     F8001040
      IA(2)=T2/100000.                                                  F8001050
C     ***** SELECT BONDS ACCORDING TO CODES *****                       F8001060
      DO 950 J=1,NCD                                                    F8001070
      JB=J                                                              F8001080
      IF(DIST-CD(1,J))    950,880,880                                   F8001090
  880 IF(CD(2,J)-DIST)    950,881,881                                   F8001100
  881 DO 885 K=1,2                                                      F8001110
      IF(IA(K)-KD(1,J))   885,882,882                                   F8001120
  882 IF(KD(2,J)-IA(K))   885,883,883                                   F8001130
  883 IF(IA(K+1)-KD(3,J))885,884,884                                    F8001140
  884 IF(KD(4,J)-IA(K+1))885,890,890                                    F8001150
  885 CONTINUE                                                          F8001160
      GO TO 950                                                         F8001170
C     ***** CHECK FOR POLYHEDRA CODE *****                              F8001180
  890 IF(CD(8,J))900,955,955                                            F8001190
  900 U1(4)=ATOMS(2,M)                                                  F8001200
      U1(5)=ATOMS(3,M)                                                  F8001210
      U1(6)=ATOMS(4,M)                                                  F8001220
      KN1=ABS(CD(4,J))                                                  F8001230
      KN2=ABS(CD(5,J))                                                  F8001240
      DSQ1=(CD(6,J))**2                                                 F8001250
      DSQ2=(CD(7,J))**2                                                 F8001260
C     ***** SEARCH FOR POLYHEDRA CENTER *****                           F8001270
      DO 935 IN=1,LATM                                                  F8001280
      K3=ATOMS(1,IN)/100000.                                            F8001290
      IF(K3-KN1) 935,905,905                                            F8001300
  905 IF(KN2-K3) 935,910,910                                            F8001310
C     ***** CHECK POLYHEDRA DISTANCE RANGE *****                        F8001320
  910 DO 930 J1=1,4,3                                                   F8001330
      DSQ=(ATOMS(2,IN)-U1(J1))**2                                       F8001340
      IF(DSQ2-DSQ) 935,915,915                                          F8001350
  915 DSQ=DSQ+(ATOMS(3,IN)-U1(J1+1))**2                                 F8001360
      IF(DSQ2-DSQ) 935,920,920                                          F8001370
  920 DSQ=DSQ+(ATOMS(4,IN)-U1(J1+2))**2                                 F8001380
      IF(DSQ2-DSQ) 935,925,925                                          F8001390
  925 IF(DSQ-DSQ1) 935,930,930                                          F8001400
  930 CONTINUE                                                          F8001410
      GO TO 955                                                         F8001420
  935 CONTINUE                                                          F8001430
C     ***** END OF POLYHEDRA CHECK *****                                F8001440
  950 CONTINUE                                                          F8001450
      GO TO 975                                                         F8001460
C     ***** PREPARE TO DRAW BOND *****                                  F8001470
  955 IF(NJ2-10) 960,970,970                                            F8001480
  960 LNS=MOD(LNS+1,56)                                                 F8001490
      IF(LNS) 965,965,970                                               F8001500
  965 WRITE (NOUT,835) (TITLE(I),I=1,18)                                F8001510
      WRITE (NOUT,837)                                                  F8001520
  970 CALL BOND(T1,T2,JB,NA1,NA2)                                       F8001530
  975 CONTINUE                                                          F8001540
  977 CONTINUE                                                          F8001550
C     ***** ELIMINATE LOCAL OVERLAP INFORMATION BEFORE RETURNING *****  F8001560
  980 IF(NJ2-21) 985,990,990                                            F8001570
  985 CALL LAP900(-1)                                                   F8001580
  990 RETURN                                                            F8001590
      END                                                               F8001600

      SUBROUTINE F900                                                   F900  10
      DIMENSION X(3),YO(3,3),Y(3),Z(3)                                  F900  20
      REAL*8 CHEM                                                       F900  30
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    F900  40
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(160),CONT(5),D(3,130)F900  50
      DIMENSION DA(3,3),DP(2,130),EV(3,160),FS(3,3,80),KD(5,10),ORGN(3) F900  60
      DIMENSION P(3,160),PA(3,3,160),PAC(3,4),PAT(3,3),Q(3,3),REFV(3,3) F900  70
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,48)   F900  80
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   F900  90
      DIMENSION XLNG(3),XO(3),XT(3)                                     F900 100
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BBOX,CD,CHEM,CONT,D   F900 110
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LINO,NATOM,NCD F900 120
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1F900 130
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   F900 140
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      COMMON V3,V4,V5,V6,UNIT,XLNG,XO,XT                                F900 150
C     ***** LABELLING FUNCTION SUBROUTINE *****                         F900 160
      ITILT=0                                                           F900 170
      NJ3=MOD(NJ2,10)                                                   F900 180
      TH=THETA                                                          F900 190
      SINTH=SYMB(2,1)                                                   F900 200
      COSTH=SYMB(1,1)                                                   F900 210
      ILAST=1                                                           F900 220
      IF(AIN(2)-11100.)910,910,905                                      F900 230
  905 ILAST=2                                                           F900 240
  910 DO 925 II=1,ILAST                                                 F900 250
C     ***** OBTAIN WORKING CARTESIAN COORDINATES *****                  F900 260
      CALL XYZ(AIN(II),XU(1,II),2)                                      F900 270
      IF(NG)915,925,915                                                 F900 280
  912 NG=11                                                             F900 290
  915 CALL ERPNT(AIN(II),NJ3*100+NJ2)                                   F900 300
      GO TO 1190                                                        F900 310
  925 CALL XYZ(AIN(II),XU(1,II+3),3)                                    F900 320
      II=1                                                              F900 330
C     ***** FIND MEAN REFERENCE POINT *****                             F900 340
      DO 930 J=1,3                                                      F900 350
      T2=XU(J,ILAST)                                                    F900 360
      T1=XU(J,1)                                                        F900 370
      XU(J,3)=T2-T1                                                     F900 380
  930 X(J)=(T2+T1)*0.5                                                  F900 390
C     ***** PERSPECTIVE SCALING FACTOR *****                            F900 400
      SCAL=1.                                                           F900 410
      IF(VIEW)940,940,935                                               F900 420
  935 SCAL=VIEW/(VIEW-X(3))                                             F900 430
  940 HGT=SCAL*AIN(5)                                                   F900 440
      IF(NJ2-3)960,950,945                                              F900 450
  945 IF(NJ2-8)950,950,960                                              F900 460
C     ***** PROJECTED VECTOR BASELINE *****                             F900 470
  950 CALL PLTXY(XU(1,4),V1)                                            F900 480
      CALL PLTXY(XU(1,5),V2)                                            F900 490
      T1=V2(1)-V1(1)                                                    F900 500
      T2=V2(2)-V1(2)                                                    F900 510
      T3=SQRT(T1*T1+T2*T2)                                              F900 520
      IF(T3)912,912,955                                                 F900 530
  955 COSTH=T1/T3                                                       F900 540
      SINTH=T2/T3                                                       F900 550
      TH=ARCCOS(COSTH)                                                  F900 560
      IF(SINTH)958,960,960                                              F900 570
  958 TH=-TH                                                            F900 580
  960 IF(NJ2-11)965,985,985                                             F900 590
C     ***** FIND CENTER OF PROJECTED LABEL *****                        F900 600
  965 Y(1)=SCAL*(X(1)+AIN(6)*COSTH-AIN(7)*SINTH)+XO(1)                  F900 610
      Y(2)=SCAL*(X(2)+AIN(6)*SINTH+AIN(7)*COSTH)+XO(2)                  F900 620
      Y(3)=0.                                                           F900 630
C     ***** CHECK FOR LEGEND RESET *****                                F900 640
      DO 980 J=1,2                                                      F900 650
      T1=AIN(J+2)                                                       F900 660
      IF(T1)975,980,970                                                 F900 670
  970 Y(J)=T1                                                           F900 680
      GO TO 980                                                         F900 690
  975 Y(J)=XLNG(J)+T1                                                   F900 700
  980 CONTINUE                                                          F900 710
C     ***** SET PARAMETERS FOR INDIVIDUAL FUNCTIONS *****               F900 720
  985 GO TO(990,995,995,1000,1300,1000,915,1105,1105,915,915,915,1305,10F900 730
     105,1305,1005,915),NJ3                                             F900 740
  990 TH=0.                                                             F900 750
      L=AIN(1)/100000.                                                  F900 760
      ILAST=1                                                           F900 770
      DXU=0.                                                            F900 780
      DYU=0.                                                            F900 790
      GO TO 1030                                                        F900 800
  995 TH=270.                                                           F900 810
      ILAST=10                                                          F900 820
      T1=HGT*28./7.                                                     F900 830
      DXU=COSTH*HGT1                                                    F900 840
      DYU=SINTH*HGT1                                                    F900 850
      GO TO 1030                                                        F900 860
 1000 TH=10*10*(NJ3-6)                                                  F900 870
      DIST=SQRT(VM(XU(1,1),XU(1,4)))/SCAL1                              F900 880
      GO TO 1310                                                        F900 890
C     ***** TEST PERSPECTIVE LABELS *****                               F900 900
 1005 CALL DOT1(XU(1,3),VT(1,1),1)                                      F900 910
      IF(ABS(VT(1,1))-.9999)1315,912,912                                F900 920
C     ***** FORM PERSPECTIVE ROTATION MATRIX *****                      F900 930
 1310 CALL NORM(AID(1,1),VT(1,1),VT(1,2),1)                             F900 940
      CALL NORM(VT(1,2),VT(1,3),1)                                      F900 950
      CALL UNORM(VT(1,1),VT(1,2),VT(1,3),1)                             F900 960
      DO 1315 J=1,3                                                     F900 970
 1315 VT(J,4)=X(J)                                                      F900 980
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      ITILT=1                                                           F900 990
      HGT=AIN(5)                                                        F9001000
      TH=0.                                                             F9001010
      Y(1)=X(1)                                                         F9001020
      Y(2)=X(2)+AIN(7)-HGT*.5                                           F9001030
      IF(NJ3-13)1030,1025,1020                                          F9001040
C     ***** PERSPECTIVE BOND LABELS *****                               F9001050
 1020 Y(1)=X(1)+AIN(6)-HGT*FLOAT(22+3*(6-NJ3)))/7.                      F9001060
      DIST=SQRT(VM(XU(1,3),XU(1,3)))/SCAL1                              F9001070
      GO TO 1050                                                        F9001080
C     ***** PERSPECTIVE TITLES *****                                    F9001090
 1025 Y(1)=X(1)+AIN(6)-HGT*35./7.                                       F9001100
      ILAST=10                                                          F9001110
      DXU=HGT*28./7.                                                    F9001120
      DYU=0.                                                            F9001130
      GO TO 1050                                                        F9001140
 1030 DH=HGT*4/7.                                                       F9001150
      DV=HGT*.5                                                         F9001160
      Y(1)=Y(1)-DH*COSTH+DV*SINTH                                       F9001170
      Y(2)=Y(2)-DH*SINTH-DV*COSTH                                       F9001180
      Y(3)=0.                                                           F9001190
C     ***** PLOT VARIOUS LABELS *****                                   F9001200
 1050 X(1)=Y(1)                                                         F9001210
      XO(1)=Y(1)                                                        F9001220
      GO TO(1060,1060,1060,1090,1090,1090,915,1105,1105),NJ3            F9001230
 1060 DO 1085 I=1,ILAST                                                 F9001240
      DO 1075 J=1,3,2                                                   F9001250
      X(1)=Y(1)+FLOAT(J-2)*DISP*.5                                      F9001260
      DO 1075 K=1,3,2                                                   F9001270
      X(2)=Y(2)+FLOAT(K-2)*DISP*.5                                      F9001280
      IF(NJ3-2)1065,1068,1068                                           F9001290
C     ***** PLOT CHEMICAL SYMBOL *****                                  F9001300
 1065 CALL SYMBOL(X(1),X(2),HGT,CHEM(L),TH,6)                           F9001310
      GO TO 1070                                                        F9001320
C     ***** PLOT TITLES *****                                           F9001330
 1068 CALL SYMBOL(X(1),X(2),HGT,TITLE2(I),TH,8)                         F9001340
 1070 IF(DISP)1080,1080,1075                                            F9001350
 1075 CONTINUE                                                          F9001360
 1080 Y(1)=Y(1)+DXU                                                     F9001370
 1085 Y(2)=Y(2)+DYU                                                     F9001380
      GO TO 1190                                                        F9001390
C     ***** PLOT BOND DISTANCE LABELS *****                             F9001400
 1090 T9=NJ3-3                                                          F9001410
      T9=10.**T9                                                        F9001420
      DISTR=AINT((DIST*T9)+0.5)/T9 +.0001                               F9001430
      CALL NUMBER(Y(1),Y(2),HGT,DISTR,TH,T9)                            F9001440
      GO TO 1190                                                        F9001450
C     ***** PLOT CENTERED SYMBOLS *****                                 F9001460
 1105 CALL SYMBOL(Y(1),Y(2),HGT, IPIX(AIN(8)),TH,7-NJ3)                 F9001470
 1190 ITILT=0                                                           F9001480
      RETURN                                                            F9001490
      END                                                               F9001500


      SUBROUTINE F100                                                   F100  10
      DIMENSION DA(3,3),D15(15),DEL(3,3),DQ(6),QC(6)                    F100  20
      DIMENSION C1(3),QP(3,3),CT(10),CE(10)                             F100  30
      DIMENSION CIJK(3,3,3),GAMMA(3,3,3),D2(3,3),D1(3,3)                F100  40
      DIMENSION TA(3),T1(3),T2(3),WS0(3),WS1(3),ITBL(22,2),NTAB(22)     F100  50
      REAL*8 CHEM                                                       F100  60
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    F100  70
      DIMENSION ATOMS(8,500),BB(3,3),CD(8,10),CHEM(505),CONT(5),D(3,110)F100  80
      DIMENSION EE(3,3),DP(3,110),EV(3,168),FS(3,3,48),SD(5,10),ORGO(3) F100  90
      DIMENSION P(3,168),PA(3,3,168),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) F100 100
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,48)   F100 110
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),UNIT(3,3)   F100 120
      DIMENSION XLNG(3),XO(3),XT(3)                                     F100 130
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BBPO,CD,CHEM,CONT,D   F100 140
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTOC,NATOM,NCD F100 150
      COMMON NJ,NJ2,NOUT,NW,NSYM,ORGO,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1F100 160
      COMMON SCAL2,SPD,SYMB,TAPED,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   F100 170
      COMMON V3,V4,V5,V6,UNIT,XLNG,XO,XT                                F100 180
      EQUIVALENCE (LTOC(1),NTAB(1))                                     F100 190
C**** SUBROUTINE TO ANALYZE TENSORS OF HIGHER CUMULANTS ****             F100 200
C     COLUMN  4- 9  = 1000                                              F100 210
C     COLUMN 10-18 FIRST ATOM WITH SKEW TENSOR, IF 0 OR BLANK IS SET = 1F100 220
C     COLUMN 19-27 LAST ATOM WITH SKEW TENSOR, IF ZERO IS SET = NATOM   F100 230
C     COLUMN 28-36 IF ZERO SHIFT POSITION PARAMETERS OF ATOM TO ORIG    F100 240
C                  IF .GT. ZERO, DO NOT SHIFT TO ORIG                   F100 250
C     COLUMN 37-45 PSI AND CHI IF ZERO, ONLY PSI IF 1, ONLY CHI IF =2   F100 260
C**** CONTINUATION CARD IF A 1 IN COLUMN 3 OF PREVIOUS CARD ****        F100 270
C     COLUMN 10-18 SCALE FACTOR FOR MAPS, IF ZERO, = 0.05               F100 280
C     COLUMN 19-27 NUMBER OF GRID POINTS ALONG X IS 41                  F100 290
C     COLUMN 28-36                             Y                        F100 300
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C     COLUMN 41-45                        X                          F100 310
C     COLUMN 46-50  INCREMENT ALONG X IN ANGSTROMS                   F100 320
C     COLUMN 51-55                        Y                          F100 330
C     COLUMN 56-60                        Z                          F100 340
C**** CONTINUATION CARD IF A 1 IN COLUMN 1 OF PREVIOUS CARD ****    F100 350
C     COLUMN 10-18  [illegible] TO POINT OF X                        F100 360
C     COLUMN 19-27                            Y                      F100 370
C     COLUMN 28-36                            Z                      F100 380
C     COLUMN 37-40  NON-ZERO TO READ AND SUBTRACT RIGID-BODY CUMULANTS  F100 390
C     COLUMN 41-50  SCALE FACTOR FOR REGULAR    CUMULANTS IN SUBTRACTION F100 400
C     COLUMN 51-60  SCALE FACTOR FOR RIGID BODY CUMULANTS IN SUBTRACTION F100 410
C     COLUMN 61-72  NON-ZERO TO READ OLD FORMAT CIJK(I,J,K) CARDS    F100 420
      NA1 = ATV(1)                                                   F100 430
      IF(NA1)205,200,205                                             F100 440
  200 NA1 = 1                                                        F100 450
  205 NA2 = ATV(2)                                                   F100 460
      IF(NA2)210,210,215                                             F100 470
  210 NA2 = NATOM                                                    F100 480
  215 DO 595 IA = NA1,NA2                                            F100 490
C     ***** READ IN FIRST AND SECOND CUMULANT TENSORS *****          F100 500
      READ(IU,2) CONST,SCAT,FRAC,(V5(J),J=1,3),D2(1,1),D2(2,2),D2(3,3) F100 510
     1,D2(1,2),D2(1,3),D2(2,3),ALPHA,IOB,ICG,IDL                     F100 520
    2 FORMAT (A6,1X,5F9.5,24X / 6F9.6,F7.0,2X,3I1)                   F100 530
      CONST=0.501                                                    F100 533
      IF(ATV(23))2152,2152,2151                                      F100 536
 2151 CONST=1./01.10170                                              F100 540
      GO TO 229                                                      F100 543
 2152 IF(ICG-1)222,217,216                                           F100 546
  216 IF(ICG-1)220,217,220                                           F100 550
C     ***** READ CONTRACTED GAMMA TENSOR (COVARIANT FORM) *****      F100 560
  217 READ (IU,4)(C1(J),J=1,3)                                       F100 570
    4 FORMAT (3F10.7,10X)                                            F100 580
      ICG=1                                                          F100 590
      GO TO 222                                                      F100 600
C     ***** READ FULL GAMMA TENSOR (CONTRAVARIANT FORM) *****        F100 610
  220 READ (IU,4)(CIJK(1,1,1),CIJK(2,2,2),CIJK(3,3,3),CIJK(1,1,2)   F100 620
     1,CIJK(1,2,2),CIJK(1,1,3),CIJK(1,3,3),CIJK(2,2,3),CIJK(2,3,3)  F100 630
     2,CIJK(1,2,3))                                                  F100 640
      ICG=10                                                         F100 650
  222 IF(IDL-1)201,225,221                                           F100 660
  221 IF(IDL-6)224,226,224                                           F100 670
  224 IF(IDL-15)224,227,201                                          F100 680
C     ***** READ DELTA TENSOR *****                                  F100 690
  225 READ (IU,4) D1                                                 F100 700
      IDL=1                                                          F100 710
      GO TO 201                                                      F100 720
  226 READ (IU,4) D6(1,1),D6(2,2),D6(3,3),D6(1,2),D6(1,3),D6(2,3)   F100 730
      IDL=6                                                          F100 740
      GO TO 201                                                      F100 750
  227 READ (IU,4) D15(1),D15(11),D15(15),D15(2),D15(7),D15(3),D15(10) F100 760
     1,D15(12),D15(14),D15(6),D15(4),D15(13),D15(5),D15(8),D15(9)    F100 770
      IDL=15                                                         F100 780
C     ***** EXPAND DELTA2 TENSOR, MULTIPLY BY 2 / (8 * PI**2) *****  F100 790
  201 DO 202 I=1,3                                                   F100 800
      DO 202 J=I,3                                                   F100 810
      D2(I,J)=D2(I,J)*5.06605918E-2                                  F100 820
  202 D2(J,I)=D2(I,J)                                                F100 830
      IF(ICG-1)2901,203,207                                          F100 840
  203 IF(ALPHA)500,500,200                                           F100 850
C     ***** EXPAND CONTRACTED GAMMA TENSOR *****                     F100 860
  200 T1=0.25/ALPHA**2                                               F100 870
      DO 205 J=1,3                                                   F100 880
  205 V2(J)=C1(J)*T1                                                 F100 890
      CALL MV(D2,V2,C1)                                              F100 900
      DO 206 I=1,3                                                   F100 910
      DO 206 J=I,3                                                   F100 920
      DO 206 K=J,3                                                   F100 930
  206 CIJK(I,J,K)= C1(I)*D2(J,K)+C1(K)*D2(I,J)+C1(J)*D2(K,I)        F100 940
  207 IF(ATV(10))219,209,219                                         F100 950
C     ***** READ AND SUBTRACT OUT RIGID-BODY CONTRIBUTION *****      F100 960
  219 READ(IU,2)CONST,SCAT,FRAC,(V5(J),J=1,3),D1(1,1),D1(2,2),D1(3,3) F100 970
     1,D1(1,2),D1(1,3),D1(2,3)                                       F100 980
      READ (IU,4)                                                    F100 990
     1GAMMA(1,1,1),GAMMA(2,2,2),GAMMA(3,3,3),GAMMA(1,1,2),GAMMA(1,2,2) F1001000
     2,GAMMA(1,1,3),GAMMA(1,3,3),GAMMA(2,2,3),GAMMA(2,3,3),GAMMA(1,2,3) F1001010
      DO 208 I = 1,3                                                 F1001020
      DO 208 J = I,3                                                 F1001030
      DO 208 K = J,3                                                 F1001040
  208 CIJK(I,J,K) = CIJK(I,J,K)*ATV(10)-GAMMA(I,J,K)*ATV(20)        F1001050
  209 DO 250 I=1,3                                                   F1001060
      DO 250 J=I,3                                                   F1001070
      DO 250 K = J,3                                                 F1001080
      T1 = CIJK(I,J,K)*CONST                                         F1001090
      CIJK(I,J,K) = T1                                               F1001100
      CIJK(K,I,J) = T1                                               F1001110
      CIJK(J,K,I) = T1                                               F1001120
      CIJK(K,J,I) = T1                                               F1001130
      CIJK(I,K,J) = T1                                               F1001140
  250 CIJK(J,I,K) = T1                                               F1001150
C     ***** EXPAND CONTRACTED DELTA TENSORS *****                    F1001160
 2501 IF(IDL-1)260,251,253                                           F1001170
  251 D1=D1*24.0                                                     F1001180
      DO 252 I=1,3                                                   F1001190
      DO 252 J=1,3                                                   F1001200
  252 D6(I,J)=D2(I,J)*D1/2.0                                         F1001210
  253 IF(IDL-6)256,256,260                                           F1001220
C     ***** CONVERT TO CONTRAVARIANT FORM *****                      F1001230
  256 T1=24./(ALPHA**4)                                              F1001240
      DO 255 I=1,3                                                   F1001250
      DO 255 J=I,3                                                   F1001260
      DAL(I,J)=D6(I,J)*T1                                            F1001270
  255 DAL(J,I)=DAL(I,J)                                              F1001280
      CALL MM(D2,DAL,DA)                                             F1001290
      CALL MM(DA,D2,D6)                                              F1001300
C     ***** EXPAND TO 4TH ORDER TENSOR *****                         F1001310
  258 IJKL=0                                                         F1001320
      DO 257 I=1,3                                                   F1001330
      DO 257 J=I,3                                                   F1001340
      DO 257 K=J,3                                                   F1001350
      DO 257 L=K,3                                                   F1001360
      IJKL=IJKL+1                                                    F1001370
  257 D15(IJKL)=(D2(I,J)*D6(K,L)+D2(I,K)*D6(J,L)+D2(I,L)*D6(J,K)    F1001380
     1           +D2(K,L)*D6(I,J)+D2(J,L)*D6(I,K)+D2(J,K)*D6(I,L))/6.0 F1001390
C     ***** INVERT BETA MATRIX *****                                 F1001400
  260 CALL PAPPS(FLOAT(IA)*100000.+55501.,1)                         F1001410
C     ***** STORE IN ARRAY WITH PROPER MULTIPLICITY *****            F1001420
      IJ=0                                                           F1001430
      DO 262 I=1,3                                                   F1001440
      DO 262 J=I,3                                                   F1001450
      IJ=IJ+1                                                        F1001460
      T1=2.0                                                         F1001470
      IF(I-J)262,261,262                                             F1001480
  261 T1=1.0                                                         F1001490
  262 QQ(IJ)=Q(I,J)*T1                                               F1001500
      IF(IDL-6)270,267,263                                           F1001510
C     ***** CONTRACT 4TH ORDER DELTA TENSOR *****                    F1001520
  263 IJ=0                                                           F1001530
      DO 265 I=1,3                                                   F1001540
      DO 265 J=I,3                                                   F1001550
      IJ=IJ+1                                                        F1001560
      DQ(IJ)=0.0                                                     F1001570
      M=IJ-1                                                         F1001580
      KL=0                                                           F1001590
      DO 265 K=1,3                                                   F1001600
      [illegible]                                                    F1001610
      DO 265 L=K,3                                                   F1001620
      KL=KL+1                                                        F1001630
      M=M+1                                                          F1001640
  265 DQ(IJ)=DQ(IJ) + QQ(KL)*D15(M)                                  F1001650
      IJ=0                                                           F1001660
      DO 266 I=1,3                                                   F1001670
      DO 266 J=I,3                                                   F1001680
      IJ=IJ+1                                                        F1001690
      D6(I,J)=DQ(IJ)                                                 F1001700
  266 D6(J,I)=DQ(IJ)                                                 F1001710
C     ***** CONTRACT 2ND ORDER DELTA TENSOR                          F1001720
  267 D1=0.0                                                         F1001730
      DO 268 I=1,3                                                   F1001740
      DO 268 J=1,3                                                   F1001750
  268 D1=D1+Q(I,J)*D6(I,J)                                           F1001760
  270 IF(ICG-1)500,275,275                                           F1001770
C     ***** CONTRACT GAMMA TENSOR *****                              F1001780
  275 DO 285 K = 1,3                                                 F1001790
      T1 = 0.0                                                       F1001800
      DO 280 J = 1,3                                                 F1001810
      VT(K,J) = Q6(K,J,IA)/RV(J,IA)                                  F1001820
      DO 280 I = 1,3                                                 F1001830
  280 T1 = T1 + CIJK(I,J,K)* Q(I,J)                                  F1001840
  285 V1(K) = T1                                                     F1001850
      DO 290 J = 1,3                                                 F1001860
C     ***** PUSH FIRST CUMULANT - MEAN DIFFERENCE VECTOR IN V5 *****  F1001870
      V5(J) = V6(J) - P(J,IA) + 0.5 * ALPHA * V1(J)                  F1001880
      V8(J) = RV(J,IA)**2                                            F1001890
  290 V3(J) = 1.0 / V8(J)                                            F1001900
      WRITE(NOUT,8) (TITLE(I),I=1,18)                                F1001910
    8 FORMAT(1H1,10X,18A4)                                           F1001920
      WRITE (NOUT,10)                                                F1001930
   10 FORMAT(1H0, 9H NO. ATOM,5X,5HSIL(1),6X,5HSIL(2),6X,5HSIL(3),  1X,33H(F1001940
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     1CONTRACTED M(I,J,K) -   M(IJK) =,1X,5HM(1),6X,5HM(2),6X,5HM(3)/P1001950
     2 1H ,10X,7HM(111),6X,7HM(222),6X,7HM(333),6X,7HM(112),6X,         P1001960
     37HM(122),6X,7HM(113),6X,7HM(133),6X,7HM(223),6X,7HM(233),6X,      P1001970
     47HM(123))                                                         P1001980
      WRITE (NOUT,12)                                                   P1001990
   12 FORMAT(1H0,22HCRYSTAL OBLIQUE SYSTEM)                             P1002000
      WRITE (NOUT,10) IA,CHEM(IA),(V1(J),J=1,3),(V1(J),J=1,3),          P1002010
     1C1JK(1,1,1),C1JK(2,2,2),C1JK(3,3,3),C1JK(1,1,2),C1JK(1,2,2),      P1002020
     2C1JK(1,1,3),C1JK(1,3,3),C1JK(2,2,3),C1JK(2,3,3),C1JK(1,2,3)       P1002030
   10 FORMAT(1H ,I3,1X,A6,1P11.4,1X,1P11.4/1H ,10X,1P11.4,F10.4)        P1002040
      WRITE (NOUT,14)                                                   P1002050
   14 FORMAT(1H0,26HREFERENCE CARTESIAN SYSTEM)                         P1002060
C     ***** TRANSFORMATION MATRIX FOR REFERENCE CARTESIAN SYSTEM *****  P1002070
      DO 205 J = 1,9                                                    P1002080
  205 PAC(J,1) = AAVE(J,1)                                              P1002090
      ISTR = 0                                                          P1002100
      GO TO 105                                                         P1002110
C     ***** REPLACE REFERENCE SYSTEM BY PRINCIPAL AXIS SYSTEM *****     P1002120
  100 CALL VMJ(AA,VV,PAC)                                               P1002130
      WRITE (NOUT,16)                                                   P1002140
   16 FORMAT(1H0,15HUNIT VARIANCE PRINCIPAL-AXIS SYSTEM)                P1002150
C     ***** TRANSFORM GAMMA TENSOR TO ORTHOGONAL SYSTEM *****           P1002160
  105 DO 115 N = 1,3                                                    P1002170
      DO 115 M = N,3                                                    P1002180
      DO 115 L = M,3                                                    P1002190
      T1 = 0.0                                                          P1002200
      DO 112 K = 1,3                                                    P1002210
      T2 = PAC(K,N)                                                     P1002220
      DO 112 J = 1,3                                                    P1002230
      T3 = T2 * PAC(J,M)                                                P1002240
      DO 110 I = 1,3                                                    P1002250
  110 T1 = T1 + C1JK(I,J,K)*PAC(I,L)*T3                                 P1002260
      GAMMA(L,M,N) = T1                                                 P1002270
      GAMMA(M,L,N) = T1                                                 P1002280
      GAMMA(N,M,L) = T1                                                 P1002290
      GAMMA(M,N,L) = T1                                                 P1002300
      GAMMA(L,N,M) = T1                                                 P1002310
  115 GAMMA(N,L,M) = T1                                                 P1002320
C     ***** TRANSFORM VECTORS TO ORTHOGONAL SYSTEM *****                P1002330
      DO 120 J = 1,3                                                    P1002340
      V2(J) = 0.0                                                       P1002350
      V6(J) = 0.0                                                       P1002360
      V4(J) = 0.0                                                       P1002370
      DO 120 I = 1,3                                                    P1002380
      V6(J) = V6(J) + V1(I)*PAC(I,J)                                    P1002390
  120 V4(J) = V4(J) + V5(I)*PAC(I,J)                                    P1002400
  125 WRITE (NOUT,20) IA,CHEM(IA),(V6(J),J=1,3),(V4(J),J=1,3)           P1002410
     1,GAMMA(1,1,1),GAMMA(2,2,2),GAMMA(3,3,3),GAMMA(1,1,2),GAMMA(1,2,2) P1002420
     2,GAMMA(1,1,3),GAMMA(1,3,3),GAMMA(2,2,3),GAMMA(2,3,3),GAMMA(1,2,3) P1002430
   20 FORMAT(1H ,I3,1X,A6,1P11.4,1X,1P11.4/1H ,10X,1P11.4,F10.4)        P1002440
      IF(ISTR) 117 ,130 ,107                                            P1002450
C     ***** STORE M(IJK), M(I,J,K) AND INVERSE OF M(I,J) FOR PDGE SYSTEMP1002460
  117 CALL PATTY(FLOAT(IA)*100000.+55501.,1)                            P1002470
      IJK = 1                                                           P1002480
      DO 115  I = 1,3                                                   P1002490
      C1(I) = V6(I)                                                     P1002500
      DO 115  J = I,3                                                   P1002510
      PP(J,I) = Q(J,I)                                                  P1002520
      PP(I,J) = Q(I,J)                                                  P1002530
      DO 115  K = J,3                                                   P1002540
      C1(IJK) = GAMMA(I,J,K)*6.0                                        P1002550
  115 IJK = IJK + 1                                                     P1002560
      C1(5) = C1(5)/2.0                                                 P1002570
      C1(7) = C1(7)/2.0                                                 P1002580
      C1(10) = C1(10)/2.0                                               P1002590
      C1(8) = C1(8)*2.0                                                 P1002600
      CALL PATTY(FLOAT(IA)*100000.+55501.,-1)                           P1002610
      GO TO 153                                                         P1002620
  160 DO 165 I = 1,9                                                    P1002630
  165 Q(I,1) = AT(I,1)                                                  P1002640
C     ***** EXPAND THE CONTRACTED VECTOR *****                          P1002650
  150 IJK = 1                                                           P1002660
      DO 155 I = 1,3                                                    P1002670
      DO 155 J = I,3                                                    P1002680
      DO 155 K = J,3                                                    P1002690
      CE(IJK) = 6.0*(V4(I)*Q(J,K)+V4(J)*Q(K,I)+V4(K)*Q(I,J))            P1002700
  155 IJK = IJK + 1                                                     P1002710
      WRITE (NOUT,22) CE(1),CE(5),CE(10),CE(2),CE(4),CE(3),CE(6),CE(9)  P1002720
     1,CE(8),CE(7)                                                      P1002730
   22 FORMAT(1H FOUR M(IJK),1P11.4,F10.4)                               P1002740
      ISTR = ISTR + 1                                                   P1002750
      IF(ISTR-1) 100,100,160                                            P1002760
C     ***** MULTIPLY TERMS IN BASIC UNIT OF GAMMA BY THEIR MULTIPLICITY P1002770
  160 GAMMA(1,1,2) = GAMMA(1,1,2)*3.0                                   P1002780
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      GAMMA(1,2,2) = GAMMA(1,2,2)*3.0                                   P1002790
      GAMMA(1,1,3) = GAMMA(1,1,3)*3.0                                   P1002800
      GAMMA(1,3,3) = GAMMA(1,3,3)*3.0                                   P1002810
      GAMMA(2,2,3) = GAMMA(2,2,3)*3.0                                   P1002820
      GAMMA(2,3,3) = GAMMA(2,3,3)*3.0                                   P1002830
      GAMMA(1,2,3) = GAMMA(1,2,3)*6.0                                   P1002840
C     ***** CALCULATE MODE OF PROBABILITY DENSITY FUNCTION *****        P1002850
      T4 = 0.0                                                          P1002860
      DO 165 J = 1,3                                                    P1002870
      V2(J) = V4(J)-V6(J)*0.5                                           P1002880
  165 T4 = T4 + V2(J)**2                                                P1002890
      T4 = SQRT(T4)                                                     P1002900
      IF(T4-1.0) 180,180,170                                            P1002910
  170 DO 175 J = 1,3                                                    P1002920
  175 V2(J) = V2(J)/T4                                                  P1002930
  180 CALL NEWRIT(V2,V6,GAMMA,OUT,CHI,BV(1,IA),1)                       P1002940
      T4 = 0.0                                                          P1002950
      DO 185 J = 1,3                                                    P1002960
      T1 = BT(J,IA)                                                     P1002970
      V2(J) = V2(J)*T1                                                  P1002980
  185 T4 = T4 + V2(J)**2                                                P1002990
      T4 = SQRT(T4)                                                     P1003000
C     ***** SHIFT POSITIONAL PARAMETERS TO MODE *****                   P1003010
      DO 195 J = 1,3                                                    P1003020
      V5(J) = P(J,IA)                                                   P1003030
      V7(J) = V5(J)                                                     P1003040
      DO 190 I = 1,3                                                    P1003050
  190 P(J,IA) = P(J,IA) + V2(I)*PA(J,I,IA)                              P1003060
  195 V1(J) = P(J,IA) - V5(J)                                           P1003070
      WRITE (NOUT,26)                                                   P1003080
   26 FORMAT(1H0,15X,6HX MEAN,5X,6HY MEAN,5X,6HZ MEAN,16X,6HX MODE,5X,  P1003090
     16HY MODE,5X,6HZ MODE,20X,12HDISPLACEMENT)                         P1003100
      WRITE (NOUT,32)                                                   P1003110
      WRITE (NOUT,26) IA,CHEM(IA),(V5(J),J=1,3),(V7(J),J=1,3),T4        P1003120
   26 FORMAT(1H ,I3,1X,A6,1P11.4,1X,1P11.6,16X,F6.3,1X,9HANGSTROMS)     P1003130
      T1 = 55501. + FLOAT(IA)*100000.                                   P1003140
      CALL XYZ(T1,V2,-1)                                                P1003150
      CALL XYZ(T1,V1,1)                                                 P1003160
      DO 600 J = 1,3                                                    P1003170
  600 V1(J) = V1(J) - V2(J)                                             P1003180
      IF(ATR(1)) 615,615,605                                            P1003190
  605 DO 610 J = 1,3                                                    P1003200
  610 P(J,IA) = V6(J)                                                   P1003210
      WRITE (NOUT,28)                                                   P1003220
   28 FORMAT(1H ,    29HPOSITIONAL PARAMETERS AT MEAN)                  P1003230
      GO TO 620                                                         P1003240
  615 WRITE (NOUT,40)                                                   P1003250
   40 FORMAT(1H ,    29HPOSITIONAL PARAMETERS AT MODE)                  P1003260
C     ***** PRINT MEAN AND MODE BASED ON REFERENCE CARTESIAN SYSTEM ****P1003270
  620 WRITE (NOUT,14)                                                   P1003280
      WRITE (NOUT,26) IA,CHEM(IA),(V2(J),J=1,3),(V1(J),J=1,3),T4        P1003290
C     ***** PRINT PRINCIPAL AXES BASED ON REFERENCE CARTESIAN SYSTEM ***P1003300
      WRITE (NOUT,12)                                                   P1003310
   12 FORMAT(1H0,10X,16HRMS DISPLACEMENT, 8X,11HUNIT VECTORS, BASED ON REP1003320
     1FERENCE,19X,20HCOVARIANCE MATRIX (U TENSOR))                      P1003330
      CALL PATTY(T1,-1)                                                 P1003340
      WRITE (NOUT,16) (RMS(J),(PAC(I,J),I=1,3),(U(I,J),I=1,3),J=1,3)    P1003350
   16 FORMAT(1H0,10X,F11.6,11X,1P11.6,11X,1P11.6)                       P1003360
      IF(ATR(8)) 625,505,625                                            P1003370
C     ***** CALCULATE PROBABILITY DENSITY MAP *****                     P1003380
  625 SCAT = AMAX1(SCAT,1.0)                                            P1003390
      SCALE=,06349363 *ATR(6)*SCAT/(BT(1,IA)*BT(2,IA)*BT(3,IA))         P1003400
      DO 610 I = 1,3                                                    P1003410
      DEN(J) = ATR(J+11)                                                P1003420
  610 X3(J) = ATR(J+14) - 0.5*(ATR(J+8)-1.0)*ATR(J+11)                  P1003430
      NT = ATR(9)                                                       P1003440
      NT = ATR(10)                                                      P1003450
      NR = ATR(11)                                                      P1003460
C     ***** LOOP OVER Z OF REFERENCE SYSTEM *****                       P1003470
      DO 500 IZ = 1,NZ                                                  P1003480
      DZ(1) = FLOAT(IZ)                                                 P1003490
      X1(3) = X0(3) + DZ(3)*DEN(3)                                      P1003500
      WRITE (NOUT,16) X1(3),CHEM(IA)                                    P1003510
   16 FORMAT (15H1 SECTION Z =,F6.3,1X,A6)                              P1003520
      DO 615 I = 1,NY                                                   P1003530
  615 NPART(I) = 27(2) + DX2(2)*FLOAT(I)                                P1003540
      WRITE (NOUT,10) (NPAR(I),I=1,NY)                                  P1003550
   16 FORMAT(9H Y(A,1),10,12F5.2)                                       P1003560
C     ***** LOOP OVER Y OF REFERENCE SYSTEM *****                       P1003570
      DO 495 IY = 1,NY                                                  P1003580
      DZ(2) = FLOAT(IY)                                                 P1003590
      X1(2) = X0(2) + DZ(2)*DEN(2)                                      P1003600
C     ***** LOOP OVER X OF REFERENCE SYSTEM *****                       P1003610
      DO 445 IX = 1,NX                                                  P1003620
```

```
      ZST(J) = ZINST(I)
      Z(2) = ZO(2) + ZST(J)*ZSTEP(2)
C     ***** EVALUATE ORTHONORMAL SERIES AT POINT Z(I) *****
      DO 400 I = 1,N
      Z2(I) = 0.0
      DO 400 J = 1,N
  400 Z2(I) = Z2(I) + Z(J)*EIGVEC(J,I)
      ITALLY = 1
      PSI = 0.0
      QUAD = 0.0
      DO 405 LI = 1,N
      ZZLI = Z2(LI)
      PSI = PSI + ZZLI*FIRST(LI)
      QUAD = QUAD + ZZLI*SECOND(LI)
      DO 405 LJ = LI,N
      ZZLJ = Z2(LJ)
      ZZLIZJ = ZZLI*ZZLJ - D(LI,LJ)
      DO 405 LK = LJ,N
      PSI = PSI + C(ITALLY) * (Z2(LK)*ZZLIZJ - ZZLI*D(LJ,LK)
     1- ZZLJ*D(LI,LK))
  405 ITALLY = ITALLY + 1
      PDF = SCALE*EXP(-.5*QUAD)
      CHI = PROB(PSI-1.0)
      PSI = PDF* PSI
C     ***** ROUND AND STORE PSI *****
      T1 = PSI
      LTEMP = T1 + SIGN(0.5,T1)
      IF(LTEMP)460,450,460
  450 IF(T1)455,460,460
  455 LTEMP = -0
  460 LIST(II,1) = LTEMP
C     ***** ROUND AND STORE CHI *****
      T1 = CHI
      LTEMP = T1 + SIGN(0.5,T1)
      IF(LTEMP)475,465,475
  465 IF(T1)470,475,475
  470 LTEMP = -0
  475 LIST(II,2) = LTEMP
  480 CONTINUE
C     ***** PRINT PSI AND CHI IF ITE(N).EQ.0 , ONLY PSI IF +, CHI IF - *
      IF(ITE(N))495,485,490
  485 WRITE (NOUT,80)
      WRITE (NOUT,84)Z1(I),(LIST(J,1),J=1,NT)
      WRITE (NOUT,86)Z1(I),(LIST(J,2),J=1,NT)
      GO TO 500
  490 WRITE (NOUT,82)
      WRITE (NOUT,84)Z1(I),(LIST(J,1),J=1,NT)
      GO TO 500
  495 WRITE (NOUT,82)
      WRITE (NOUT,86)Z1(I),(LIST(J,2),J=1,NT)
   80 FORMAT(1H )
   82 FORMAT(1H0)
   84 FORMAT(1H PS, F6.3,22I5)
   86 FORMAT(1H CC, F6.3,22I5)
  500 CONTINUE
  505 CONTINUE
      RETURN
      END


      SUBROUTINE HERMIT(E,D,GAMMA,PSI,CHI,DNS,ITYPE)
C     ***** SUBROUTINE TO DEFINE HERM *****
      DIMENSION E(3),D(3,3),Z(3),Y(3),GAMMA(3,3,3),H(6,3)      ,NN(10,3)
      DIMENSION  IT(5,10),IT(5),TALU(3),VECT(3,3),NN(3),B(3)
C     ***** ITYPE=0, PSI, CHI CALC/.GT.0 RETURN PSI/.LT.0 RETURN CHI
      ICYCLE = 0
      IF(ITYPE)205,200,210
  200 ASSIGN 415 TO NXT1
      ASSIGN 390 TO NXT2
      ASSIGN 415 TO NXT3
      ILAST = 1
      GO TO 220
  205 ASSIGN 415 TO NXT1
      ASSIGN 290 TO NXT2
      GO TO 215
  210 ASSIGN 310 TO NXT1
      ASSIGN 285 TO NXT2
  215 ASSIGN 300 TO NXT3
      ILAST = 0
  220 ICYCLE = ICYCLE + 1
      ASSIGN 215 TO ISRT
      ASSIGN 305 TO IRUT
      ASSIGN 270 TO I1ST
      ASSIGN 115 TO I2ST
      ASSIGN 105 TO I3ST
      HO = 1.0
C     ***** GENERATE H0,H1,....,HN FOR Z(II),II=1,N *****
      DO 230 II = 1,N
      H(1,II) = 1.0
      ZH = Z(II)
      H(2,II)
      HI = 1
      DO 225
      H(IH+1,II) = ZH*H(IH,II) - HI*H(IH-1,II)
  225 HI = HI + 1.0
      T(II) = 0.0
      NN(II) = 1
      DO 235 I = 1,N
C     ***** GENERATE HERMITE POLYNOMIALS WITHOUT (-1)**N FACTOR *****
      IH2 = IH2
      H(IH2,II) = -H(IH2,II)
  235 A(I,II) = 0.0
      NN(4) = 1
C     ***** FIND PRODUCTS OF HERMITE POLYNOMIALS *****
      DO 455 I1 = 1,ILAST
      I1M1 = I1 - 1
      IT(1) = I1M1
      NN(I1) = NN(I1) + 1
      DO 450 I2 = I1,ILAST
      I2M1 = I2 - 1
      IT(2) = I2M1
      NN(I2) = NN(I2) + 1
      DO 445 I3 = I2,N
      I3M1 = I3 - 1
      IT(3) = I3M1
      NN(I3) = NN(I3) + 1
      DO 440 I4 = I3,N
      I4M1 = I4 - 1
      IT(4) = I4M1
      NN(I4) = NN(I4) + 1
      DO 435 I5 = I4,N
      I5M1 = I5-1
      IT(5) = I5M1
      NN(I5) = NN(I5) + 1
C     *****SKIP ZERO ORDER TERM *****
      GO TO ISRT,(215,260)
  215 ASSIGN 260 TO ISRT
      GO TO 415
  260 K1 = NN(1)
      K2 = NN(2)
      K3 = NN(3)
      TERM = H(K1,1)*H(K2,2)*H(K3,3)
      GO TO IRUT,(265,285)
  265 IF(I4M1)255,255,280
  250 ASSIGN 265 TO IRUT
      GO TO 265
C     ***** USE H(I) *****
C     ***** SUM SECOND PART OF PSI *****
  255 PSI = PSI - TERM * E(I5M1)
      GO TO NXT1,(280,415)
C     ***** SUM FIRST PART OF VECTOR OF FIRST DERIVATIVES *****
  280 Y(I5M1) = Y(I5M1) - TERM
      GO TO 415
  265 GO TO I1ST,(270,105)
  270 IF(I4M1)300,300,275
  275 ASSIGN 105 TO I1ST
      GO TO 105
C     ***** USE H(I)H(J) *****
  300 GO TO NXT2,(305,290,100)
C     ***** SUM FIRST PART OF MATRIX OF SECOND DERIVATIVES *****
  285 A(I4M1,I5M1) = A(I4M1,I5M1) + TERM
C     ***** SUM SECOND PART OF VECTOR OF FIRST DERIVATIVES *****
  290 Y(I5M1) = Y(I5M1) + TERM * E(I4M1)
      IF(I5M1-I4M1)415,415,295
  295 Y(I4M1) = Y(I4M1) + TERM * E(I5M1)
      GO TO 415
C     ***** SKIP H(I)H(J) PART IF CALCULATING PSI ONLY *****
  100 NN(I5) = NN(I5) - 1
      NN(I4) = NN(I4) - 1
      GO TO 445
C     ***** CALCULATE CONSTANT*GAMMA(I,J,K)*HERMITE(I,J,K) *****
  105 TERMJ = GAMMA(I3M1,I2M1,I1M1)*TERM*0.16666667
  110 GO TO I2ST,(115,150)
  115 IF(I2M1)125,125,120
  120 ASSIGN 150 TO I2ST
      GO TO 150
```

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C     ***** USE H(I)H(J)H(K) *****                                      NEWR1070
C     ***** SUM THIRD PART OF PSI *****                                 NEWR1080
  325 PSI = PSI - TERM2                                                 NEWR1090
      GO TO NXT3,(330,435)                                              NEWR1100
C     ***** SUM SECOND PART OF MATRIX OF SECOND DERIVITIVES *****       NEWR1110
  330 A(I2N1,I5N1) = A(I2N1,I5N1) - TERM * U(I3N1)                      NEWR1120
      IF(I5N1-I2N1) 140,140,135                                         NEWR1130
  135 A(I3N1,I2N1) = A(I3N1,I2N1) - TERM * U(I5N1)                      NEWR1140
  140 IF(I2N1-I3N1)435,435,145                                          NEWR1150
  145 A(I3N1,I5N1) = A(I3N1,I5N1) - TERM * U(I2N1)                      NEWR1160
      GO TO 435                                                         NEWR1170
  150 GO TO I1NT,(155,185)                                              NEWR1180
  155 IF(I1N1) 165,165,160                                              NEWR1190
  160 ASSIGN 185 TO I1NT                                                NEWR1200
      GO TO 185                                                         NEWR1210
C     ***** USE H(I)H(J)H(K)H(L) *****                                  NEWR1220
C     ***** SUM THIRD PART OF VECTOR OF FIRST DERIVITIVES *****         NEWR1230
  165 V(I2N1) = V(I2N1) + TERM2                                         NEWR1240
      IF(I5N1-I2N1) 175,175,170                                         NEWR1250
  170 V(I5N1) = V(I5N1) + GAMMA(I2N1,I3N1,I4N1)*TERM*0.16666667         NEWR1260
  175 IF(I3N1-I5N1) 185,185,180                                         NEWR1270
  180 V(I3N1) = V(I3N1) + GAMMA(I2N1,I3N1,I5N1)*TERM*0.16666667         NEWR1280
  185 IF(I3N1-I2N1)435,435,190                                          NEWR1290
  190 V(I3N1) = V(I3N1) + GAMMA(I2N1,I4N1,I5N1)*TERM*0.16666667         NEWR1300
      GO TO 435                                                         NEWR1310
C     ***** USE H(I)H(J)H(K)H(L)H(M) *****                              NEWR1320
C     ***** SUM THIRD PART OF MATRIX OF SECOND DERIVITIVES *****        NEWR1330
C     ***** SET UP ORDERED PERMUTATIONS OF I1,I2,I3,I4,I5 BY 2 3, 1 5 **NEWR1340
  395 LT = 0                                                            NEWR1350
      LD = 11                                                           NEWR1360
      DO 410 I=1,4                                                      NEWR1370
      IP1 = I+1                                                         NEWR1380
      DO 410 J=IP1,5                                                    NEWR1390
      LT = LT+1                                                         NEWR1400
      JT(1,LT) = IT(I)                                                  NEWR1410
      JT(2,LT) = IT(J)                                                  NEWR1420
      IF(J-4)403,400,410                                                NEWR1430
  400 JP1 = J+1                                                         NEWR1440
      DO 405 K=JP1,5                                                    NEWR1450
      LD = LD-1                                                         NEWR1460
      JT(1,LD) = IT(I)                                                  NEWR1470
      JT(2,LD) = IT(J)                                                  NEWR1480
  405 JT(3,LD) = IT(K)                                                  NEWR1490
  410 CONTINUE                                                          NEWR1500
C     ***** FIND UNIQUE ORDERED PERMUTATIONS OF I1,I2,I3,I4,I5 BY 2,3 5 NEWR1510
      J1 = 0                                                            NEWR1520
      J2 = 0                                                            NEWR1530
      J3 = 0                                                            NEWR1540
      DO 430 J=1,10                                                     NEWR1550
      IF((J1-1)*(J3-1))415,435,415                                      NEWR1560
  415 IF(J1-JT(1,J))425,420,425                                         NEWR1570
  420 IF(J2-JT(2,J))425,430,425                                         NEWR1580
  425 J1 = JT(1,J)                                                      NEWR1590
      J2 = JT(2,J)                                                      NEWR1600
      J3 = JT(3,J)                                                      NEWR1610
      J4 = JT(4,J)                                                      NEWR1620
      J5 = JT(5,J)                                                      NEWR1630
      A(J1,J2) = A(J1,J2) - GAMMA(J3,J4,J5)*TERM*0.16666667             NEWR1640
  430 CONTINUE                                                          NEWR1650
  435 NH(I5) = NH(I5) - 1                                               NEWR1660
  440 NH(I4) = NH(I4) - 1                                               NEWR1670
  445 NH(I3) = NH(I3) - 1                                               NEWR1680
  450 NH(I2) = NH(I2) - 1                                               NEWR1690
  455 NH(I1) = NH(I1) - 1                                               NEWR1700
C     ***** FILL OUT MATRIX A AND MULTIPLY A,V AND PSI BY NORMAL DENSITYNEWR1710
      DEN = 0.06349363 * EXP(-.50*(X(1)**2+X(2)**2+X(3)**2))            NEWR1720
      PSI = PSI * DEN                                                   NEWR1730
      CHI = PSI - DEN                                                   NEWR1740
      IF(ITYPE)460,500,460                                              NEWR1750
C     ***** UPDATE DENSITY FOR POSITIVE MATRIX A OR MATRIX SEARCH ***** NEWR1760
  460 DEN = -DEN                                                        NEWR1770
      DO 470 I = 1,3                                                    NEWR1780
      DO 465 J = I,3                                                    NEWR1790
      A(I,J) = A(I,J)*DEN                                               NEWR1800
  465 A(J,I) = A(I,J)                                                   NEWR1810
  470 V(I) = V(I) * DEN                                                 NEWR1820
C     ***** CHECK EIGENVALUES OF MATRIX A *****                         NEWR1830
      CALL EIGEN(A,VALU,VECT)                                           NEWR1840
      IF(VALU(1))495,495,475                                            NEWR1850
C     *****CALCULATE SHIFT VECTOR *****                                 NEWR1860
  475 CALL ATP3D(A,V1,T,3)                                              NEWR1870
C     ***** CALCULATE LENGTH OF SHIFT VECTOR *****                      NEWR1880
      T1 = 0.0                                                          NEWR1890
      DO 480 J = 1,3                                                    NEWR1900
      T1 = T1 + (V1(J)*DEN(J))**2                                       NEWR1910
  480 X(J) = X(J) + V1(J)                                               NEWR1920
      IF(T1-1.0E-10)500,485,485                                         NEWR1930
C     ***** ERROR IF SHIFT IS .GT. 0.1 A *****                          NEWR1940
  485 IF(T1-0.01)490,495,495                                            NEWR1950
  490 IF(ICYCLE-20)320,495,495                                          NEWR1960
  495 PRINT 2,ICYCLE,VALU                                               NEWR1970
    2 FORMAT(32HNUMBER FAILURE ON CYCLE,I3,3E20.5)                      NEWR1980
      PRINT 6,PSI,CHI,T1,V1,X,VALU,T,A,N                                NEWR1990
    6 FORMAT(1H0/(1H ,6E19.8))                                          NEWR2000
  500 RETURN                                                            NEWR2010
      END                                                               NEWR2020

      SUBROUTINE LAPSOR(ITYPE)                                          LAPS  10
C     ***** ST  X PROJECTED ATOM CONICS AND BOND QUADRILATERALS *****   LAPS  20
      DIMENSION QC(3,3),QD(3,3),VD1(3),VD2(3)                           LAPS  30
C     ***** DOUBLE PRECISION FOR VERY SMALL ATOMS AND SHORT BONDLENGTH *LAPS  40
C     ***** IN GENERAL, DOUBLE PRECISION IS NOT REQUIRED *****          LAPS  50
      REAL*8 QC,QD,VD1,VD2,VE1,VE2,VE3                                  LAPS  60
C     ***** JUST REMOVE THE PRECEDING REAL*8 CARD TO HAVE SINGLE PREC   LAPS  70
      COMMON/OLAP/CONIC(7,500),COVER(6,30),KC(30),KQ(30),NCONIC,NCOVER, LAPS  80
     1 NQOVER,NQUAD,OVRMGN,QOVER(3,4,30),QUAD(8,600),SHAD(50,2)         LAPS  90
      REAL*8 CHIP                                                       LAPS 100
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAUNR(3,3),AID(3,3),AIN(140)    LAPS 110
      DIMENSION ATOMS(8,500),BB(3,3),CD(8,10),CHAR(144),CONT(5),D(3,110)LAPS 120
      DIMENSION DA(3,3),DP(2,110),EV(3,144),FS(3,3,80),ND(5,10),ORGN(3) LAPS 130
      DIMENSION P(3,144),PA(3,3,144),PAC(3,5),PAT(3,3),Q(3,3),REV(3,3)  LAPS 140
      DIMENSION RES(10),RMS(5),SYMM(3,3),TITLE(18),TITLE2(18),TS(3,80)  LAPS 150
      DIMENSION VT(3,4),V1(3),V2(3),V3(3),V4(3),V5(3),V6(3),VREF(3,3)   LAPS 160
      DIMENSION XLEN(3),XO(3),XT(3)                                     LAPS 170
      COMMON NG,A,AA,AAREV,AAUNR,AID,AIN,ATOMS,BB,BBDA,CD,CHAR,CONT,D   LAPS 180
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTWO,NATOM,NCD LAPS 190
      COMMON NJ,NJ2,NOUT,NSN,NSYM,ORGN,P,PA,PAC,PAT,Q,REV,RES,RMS,SCAL1LAPS 200
      COMMON SCAL2,SCL,SYMM,TAPES,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   LAPS 210
      COMMON V3,V4,V5,V6,VREF,XLEN,XO,XT                                LAPS 220
C     ***** ELIMINATE ALL PREVIOUSLY STORED LOCAL OVERLAP INFORMATION **LAPS 230
      NCOVER=0                                                          LAPS 240
      NQOVER=0                                                          LAPS 250
      IF(ITYPE)420,195,195                                              LAPS 260
C     ***** ELIMINATE ALL PREVIOUSLY STORED GLOBAL OVERLAP INFORMATION *LAPS 270
  195 NCONIC=0                                                          LAPS 280
      NQUAD=0                                                           LAPS 290
      IF(ITYPE)420,420,200                                              LAPS 300
C     ***** CONSTANT FOR OVERLAP MARGIN (UNITS MARGIN AT OVERLAP) ***** LAPS 310
  200 IF(AIN(1))205,215,210                                             LAPS 320
C     ***** NEGATIVE NUMBER OR POSITIVE INTEGER GIVES OVRMGN=0.0 *****  LAPS 330
  205 OVRMGN=0.0                                                        LAPS 340
      GO TO 225                                                         LAPS 350
C     ***** SET OVERLAP MARGIN WIDTH DIRECTLY IN INCHES *****           LAPS 360
  210 OVRMGN=AIN(1)-AINT(AIN(1))                                        LAPS 370
      GO TO 220                                                         LAPS 380
C      ***** DEFAULT OPTION, OVERLAP MARGIN WIDTH AS A FUNCTION OF SCAL1LAPS 390
  215 OVRMGN=AMAX1(SQRT(SCAL1)*0.030,0.025)                             LAPS 400
  220 WRITE (NOUT,2) OVRMGN                                             LAPS 410
    2 FORMAT(1H0,10X,17HOVERLAP MARGIN IS, F6.3,5H INCH)                LAPS 420
  225 IF(LATM)230,230,235                                               LAPS 430
  230 NG=12                                                             LAPS 440
      CALL ERPRT(0.,510+NJ2)                                            LAPS 450
      GO TO 420                                                         LAPS 460
C     ***** SORT ATOMS LIST BY -VIEWDISTANCE OR BY Z PARAMETER          LAPS 470
  235 IF(VIEW)250,250,240                                               LAPS 480
C     ***** CALCULATE VIEWDISTANCE*Z*(-1) IF VIEW.GT.ZERO *****         LAPS 490
  240 DO 245 I=1,LATM                                                   LAPS 500
      CALL XYZ(ATOMS(1,I),V1,2)                                         LAPS 510
      V1(3)=V1(3)-VIEW                                                  LAPS 520
  245 ATOMS(4,I)=-VM(V1,V1)                                             LAPS 530
      GO TO 260                                                         LAPS 540
C     ***** STORE CARTESIAN COORDINATES IF VIEW.EQ.ZERO *****           LAPS 550
  250 DO 255 I=1,LATM                                                   LAPS 560
  255 CALL XYZ(ATOMS(1,I),ATOMS(2,I),2)                                 LAPS 570
C     ***** SORTING PROCEDURE BY SHELL, COMM ACM 2,30 (1959) *****      LAPS 580
  260 M=LATM                                                            LAPS 590
  265 M=M/2                                                             LAPS 600
      IF(M)300,300,270                                                  LAPS 610
  270 K=LATM-M                                                          LAPS 620
      J=1                                                               LAPS 630
  275 I=J                                                               LAPS 640
  280 IM=I+M                                                            LAPS 650
      IF(ATOMS(4,I)-ATOMS(4,IM))295,295,285                             LAPS 660
  285 DO 290 L=1,4,1                                                    LAPS 670
      T=ATOMS(L,I)                                                      LAPS 680
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      ATOMS(L,I)=ATOMS(L,IM)
  290 ATOMS(L,IM)=T1
      I=I-M
      IF(I)295,295,280
  295 J=J+1
      IF(J-N)275,275,265
C     ***** LOOP THROUGH ALL ATOMS IN SORTED ATOMS LIST *****
  300 DO 605 IA=1,LATM
      CALL VTE(ATOMS(1,IA),ATOMS(2,IA),2)
      CALL MATRX(ATOMS(1,IA),Z)
      DO 105 J=1,3
      V1(J)=ATOMS(J+1,IA)
      VD1(J)=V1(J)
      DO 105 K=1,3
  105 QD(J,K)=Z(J,K)
      IF(VT-VU)90,100,110
C     ***** CALCULATE ENVELOPING CONE WITH ORIGIN AT VIEWPOINT *****
  110 V1(3)=V1(3)-VIEW
      VD1(3)=V1(3)
C     ***** FORM COFACTOR MATRIX *****
      DO 115 J=1,3
      J1=MOD(J,3)+1
      J2=MOD(J+1,3)+1
      DO 115 K=J,3
      K1=MOD(K,3)+1
      K2=MOD(K+1,3)+1
      QC(J,K)= QD(J1,K1)*QD(J2,K2)-QD(J1,K2)*QD(J2,K1)
  115 QC(K,J)=QC(J,K)
C     ***** FORM POLARIZED COFACTOR MATRIX AND ADD TO ELLIPSOID MATRIX *
      TD2=-SCL**2
C     ***** TD1 IS AN ARBITRARY SCALING FACTOR *****
      TD1=VMV(V1,Q,V1)
      DO 125 J=1,3
      J1=MOD(J,3)+1
      J2=MOD(J+1,3)+1
      DO 120 K=J,3
      K1=MOD(K,3)+1
      K2=MOD(K+1,3)+1
      QD(J,K)=((VD1(J2)*(QC(J1,K1)*VD1(K2)-QC(J1,K2)*VD1(K1))
     1 -VD1(J1)*(VD1(K1)*QC(J2,K2)-VD1(K2)*QC(J2,K1)))+TD2*QC(J,K))/TD1
  120 QD(K,J)=QD(J,K)
C     ***** PROJECTED ELLIPSE IN HOMOGENEOUS COORD OF WORKING SYSTEM ***
      QD(J,3)=-QD(J,3)*VIEW
  125 QD(3,J)=-QD(3,J)*VIEW
C     ***** PROJECT CENTER OF ATOM ONTO PROJECTION PLANE *****
      TD1=-VIEW/VD1(3)
      VD2(1)=VD1(1)*TD1
      VD2(2)=VD1(2)*TD1
C     ***** TRANSFORM TO NEW ORIGIN TO IMPROVE CONDITION OF MATRIX Q ***
      DO 130 J=1,3
      DO 130 K=1,2
  130 QD(J,3)=QD(J,3)+QD(J,K)*VD2(K)
      DO 135 J=1,3
      DO 135 K=1,2
  135 QD(3,J)=QD(3,J)+VD2(K)*QD(K,J)
      V6(1)=Z0(1)+VD2(1)
      V6(2)=Z0(2)+VD2(2)
      GO TO 155
C     ***** CALCULATE ENVELOPING CYLINDER ALONG Z OF WORKING SYSTEM ****
  140 DO 145 J=1,2
      DO 145 K=1,2
  145 QD(J,K)=QD(J,K)-QD(J,3)*QD(K,3)/QD(3,3)
      DO 150 J=1,2
      QD(J,3)=0.0
      QD(3,J)=0.0
  150 V6(J)=Z0(J)+ATOMS(J+1,IA)
C     ***** PROJECTED ELLIPSE IN HOMOGENEOUS COORD ABOUT CENTER OF ATOM
      QD(3,3)=-SCL**2
C     ***** FIT RECTANGLE AROUND ELLIPSE ALLOWING OVERLAP MARGIN *****
C     ***** FORM MATRIX OF COFACTORS *****
  155 DO 160 J=1,3
      J1=MOD(J,3)+1
      J2=MOD(J+1,3)+1
      DO 160 K=J,3
      K1=MOD(K,3)+1
      K2=MOD(K+1,3)+1
  160 QC(J,K)= QD(J1,K1)*QD(J2,K2)-QD(J1,K2)*QD(J2,K1)
C     ***** RESCALE MATRIX OF COFACTORS SO THAT QC(3,3)=1.0 *****
      DO 165 J=1,3
      DO 165 K=J,3
      QC(J,K)= QC(J,K)/QC(3,3)
  165 QC(K,J)=QC(J,K)
      TD2=QD(3,3)
      NDG=0
```

```
      DO 185 J=1,2
C     ***** SOLVE QUADRATIC EQUATION *****
      T1 =QC(3,J)**2-QC(J,J)
      IF(T1)170,170,175
C     ***** ROUNDOFF PROBLEMS, RESET LIMITS IN X OR Y *****
  170 NDG=1
      V5(J)=0.001+OVRMAR
      GO TO 180
  175 V5(J)= SQRT(T1)+OVRMAR
      V6(J)=V6(J)+QC(3,J)
      TD2=TD2+QD(3,J)*QC(3,J)
  180 CONIC(2*J-1,IA)=V6(J)-V5(J)
  185 CONIC(2*J,IA)=V6(J)+V5(J)
      IF(NDG)190,190,195
  190 IF(TD2)600,195,195
C     ***** ELLIPSE IMAGINARY DUE TO ROUNDOFF, RESET TO OVAL VALUE *****
  195 CONIC(5,IA)=1.0/((CONIC(2,IA)-CONIC(1,IA))*0.5)**2
      CONIC(6,IA)=0.0
      CONIC(7,IA)=1.0/((CONIC(4,IA)-CONIC(3,IA))*0.5)**2
      GO TO 605
C     ***** STORE NORMALIZED QUADRATIC COEFFICIENTS FOR ELLIPSE *****
C     ***** SCALED BY OVERLAP MARGIN PARAMETER *****
  600 TD1= -(1.0+2.0*OVRMAR/(V5(1)+V5(2)))**2 /TD2
      CONIC(5,IA)=QD(1,1)*TD1
      CONIC(6,IA)=QD(1,2)*TD1
      CONIC(7,IA)=QD(2,2)*TD1
  605 CONTINUE
      NCONIC=LATM
C     ***** PRINT OUT SORTED ATOMS ARRAY *****
      WRITE (NOUT,8) (ATOMS(1,J),J=1,LATM)
    8 FORMAT(1H0,10X,30HCONTENTS OF SORTED ATOMS ARRAY/(15X,10F10.0))
C     ***** STORE BOND QUADRANGLES IF SEARCH CODES ARE GIVEN *****
      IF(NCB)820,820,810
C     ***** GENERATE PSEUDO-INSTRUCTION #22 TO CALCULATE BONDS *****
  810 NJ2=22
      CALL FORM
      IF(NQUAD)820,820,815
C     ***** PRINT OUT NUMBER OF BOND QUADRANGLES STORED *****
C     ***** PRINT OUT QUADRANGLE IDENTIFICATION ARRAY *****
  815 WRITE (NOUT,4) NQUAD,(QUAD(9,J),J=1,NQUAD)
    4 FORMAT(1H0,10X,27HBOND OVERLAP ARRAY CONTAINS,I6,21H BONDS (MAXIMUM
     1N IS 500)/ 11X, 46HATOM-PAIR NUMBERS IN ARRAY REFER TO SEQUENCE
     2IN SORTED ATOMS ARRAY/(15X,10F10.0))
  820 RETURN
      END
```

```
      SUBROUTINE LAP700(NA,ICQ)
      DIMENSION BUTIN(3),QA(3,3,2),QC(3,3,2),V12(3,2),TRTD(2),TRAT(2)
      DIMENSION OVER(2)
C     ***** IN GENERAL, DOUBLE PRECISION IS NOT REQUIRED *****
C     ***** BUT IN CASE OF TROUBLE, ACTIVATE THE CD COMMENT CARDS *****
      REAL*8 ANG1,AOV1RQ,DOT1,ENTER,PI,PHI,POT1,POT1CN,QA,QC,QOT2,QOT2SQ
      REAL*8 DOT,TD
      COMMON/OLAP/CONIC(7,500),CNTRL(6,20),KC(20),NQ(10),NCONIC,NCNTRL,
     1 NSTRD,NQUAD,NTABLE,QOVRP(3,4,10),QUAD(9,400),STAK(50,2)
      REAL*8 CHAR
      DIMENSION A(3),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),BIN(100)
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CNTR(166),CONT(5),D(3,13)
      DIMENSION EE(3,3),DP(2,100),EV(3,100),FS(3,3,8),ID(5,10),NG(3)
      DIMENSION P(3,100),PA(3,3,100),PAC(3,3),PAT(3,3),Q(3,3),QUAT(3,3)
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(10),TITLE2(10),TS(3,96)
      DIMENSION VT(2,8),V1(3),V2(3),V3(3),V4(3),V5(3),V6(3),WORK(3,3)
      DIMENSION XLIM(3),XO(3),XT(3)
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CNTR,CONT,D
      COMMON DA,DP,DISP,EDGE,EV,FORM,FS,IN,ITILT,KD,LATM,LTPE,NATOM,NCD
      COMMON NJ,NJ2,NOUT,NPR,NRES,ORGN,P,PA,PAC,PAT,Q,QUAT,RES,RMS,SCAL1
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2
      COMMON V3,V4,V5,V6,WORK,XLIM,XO,XT
      PI=3.14159265358979323
CD    PI=3.141593
      ICQ=0
      NCNTRL=0
      NQUAD=0
      OVER(1)=OVRMAR
      OVER(2)=0.0
      IF(NCONIC-NA)200,200,205
  200 RETURN
C     ***** ROUGH CHECK FOR OVERLAPPING ATOMS *****
  205 DO 210 J=1,2
      TRTD(J)=CONIC(2*J-1,NA)
  210 TRAT(J)=CONIC(2*J,NA)
      L=0
      DO 620 IA=NA,NCONIC
```

```
      IF(IA-NA)230,230,215
  215 DO 225 J=1,2
      IF(VMAX(J)-CONIC(2*J-1,IA))820,820,220
  220 IF(VMIN(J)-CONIC(2*J,IA))225,820,820
  225 CONTINUE
C     ***** EXACT CHECK FOR OVERLAPPING ATOMS *****
  230 IF(L-1)235,235,240
  235 L=L+1
  240 CALL LAPCON(CONIC(1,IA),DA,V13(1,L),OVER(L))
      DO 245 J=1,3
      DO 245 K=1,3
  245 QA(J,K,L)=DA(J,K)
C     ***** CALCULATE COFACTORS AND DETERMINANTS *****
      DETER(L)=0.0
      DO 250 J=1,3
      J1=MOD(J,3)+1
      J2=MOD(J+1,3)+1
      DO 250 K=1,3
      K1=MOD(K,3)+1
      K2=MOD(K+1,3)+1
      TD=QA(J1,K1,L)*QA(J2,K2,L)-QA(J1,K2,L)*QA(J2,K1,L)
      DETER(L)=DETER(L)+TD*QA(J,K,L)
  250 QC(J,K,L)=TD
C     ***** DETER(L) IS THE DETERMINANT TIMES 3 *****
      IF(L-1)820,820,255
C     ***** FORM CHARACTERISTIC EQUATION AND EXAMINE ITS ROOTS *****
  255 AOV1=0.0
      BOV1=0.0
      DO 260 J=1,3
      DO 260 K=1,3
      AOV1=AOV1+QC(J,K,2)*QA(J,K,1)
  260 BOV1=BOV1+QC(J,K,1)*QA(J,K,2)
      AOV1=AOV1/ DETER(2)
      AOV1SQ=AOV1**2
      BOV1=BOV1/ DETER(2)
      POV1=BOV1-AOV1SQ
      QOV2=AOV1*(AOV1SQ-BOV1*1.5D0)+DETER(1)/(DETER(2)*2.0D0)
C5    QOV2=AOV1*(AOV1SQ-BOV1*1.5   )+DETER(1)/(DETER(2)*2.0   )
C     ***** CHECK DISCRIMINANT OF CHARACTERISTIC CUBIC EQUATION *****
      ITYPE=0
      POV1CU=POV1**3
      QOV2SQ=QOV2**2
      IF(POV1CU+QOV2SQ)270,110,265
  265 IF(POV1CU*1.00001+QOV2SQ)110,110,800
  270 IF(POV1CU+1.00001*QOV2SQ)275,110,110
C     ***** THREE REAL ROOTS, ALL DIFFERENT *****
  275 ITYPE=1
C     ***** NO INTERSECTION IF A/1 AND B/1 INVARIANTS ARE NEGATIVE *****
      IF(AOV1)280,285,285
  280 IF(BOV1)820,285,285
C     ***** CALCULATE THE ROOT OF CHARACTERISTIC CUBIC EQUATION *****
  285 IF(QOV2)295,290,295
  290 PHI=PI/2.0D0
C5290 PHI=PI/2.0
      GO TO 305
  295 PHI=DATAN(-DSQRT(-POV1CU-QOV2SQ)/QOV2)
C5295 PHI= ATAN(- SQRT(-POV1CU-QOV2SQ)/QOV2)
      IF(PHI)300,305,305
  300 PHI=PHI+PI
  305 ROOT=2.0D0*DSQRT(-POV1)*DCOS(PHI/3.0D0)-AOV1
C5305 ROOT=2.0  * SQRT(-POV1) * COS(PHI/3.0  )-AOV1
      GO TO 125
C     ***** THREE REAL ROOTS, AT LEAST TWO ARE EQUAL *****
  110 ITYPE=2
C     ***** CHECK SIGNS OF INVARIANTS A/1 AND B/1 *****
      IF(AOV1)115,120,120
  115 IF(BOV1)820,120,120
C     ***** CALCULATE REPEATED ROOT OF CUBIC EQUATION *****
  120 ROOT=DSIGN(DSQRT(-POV1),QOV2)-AOV1
C5120 ROOT= SIGN( SQRT(-POV1),QOV2)-AOV1
C     ***** FORM DEGENERATE CONIC (LINE PAIR WHICH MAY BE COINCIDENT) **
  125 DO 130 J=1,3
      DO 130 K=1,3
  130 DA(J,K)=QA(J,K,1)+ROOT*QA(J,K,2)
C     ***** EXAMINE INVARIANTS OF THE DEGENERATE CONIC *****
      T6=DA(1,1)*DA(2,2)
      T7=DA(1,2)**2
C     ***** NEGATIVE DENOTES REAL INTERSECTING LINE PAIR *****
C     ***** POSITIVE DENOTES IMAGINARY LINES INTERSECTING AT REAL POINT
      IF(T6-T7)135,165,140
  135 IF(T6*1.0001  -T7)800,165,165
  140 IF(T6-1.0001  *T7)165,165,165
  145 T6=DA(1,1)*(DA(1,1)+DA(2,2))
      T7=DA(1,3)**2+DA(2,3)**2
C     ***** NEGATIVE DENOTES REAL PARALLEL LINE PAIR *****
C     ***** POSITIVE DENOTES IMAGINARY PARALLELS *****
C     ***** ZERO DENOTES ONE REAL LINE (COINCIDENT PARALLELS) *****
      IF(T6-T7)150,160,155
  150 IF(T6*1.0001  -T7)800,160,160
  155 IF(T6-1.0001  *T7)160,160,165
C     ***** COINCIDENT LINE PAIR FOUND FOR THE REPEATED ROOT *****
  160 ITYPE=3
C     ***** COMPARE AREAS OF CONICS *****
  165 KA=1
      KB=2
      IF(QC(1,1,KA)-QC(1,1,KB))170,175,175
  170 KA=2
      KB=1
C     ***** SEE IF ONE CONIC IS INSIDE THE OTHER CONIC *****
  175 T1=0.0
      DO 185 J=1,3
      T2=QA(J,3,KB)
      DO 180 K=1,2
  180 T2=T2+QA(J,K,KB)*V13(K,KA)
  185 T1=T1+V13(J,KA)*T2
C     ***** DISCARD IF KA IS OUTSIDE KB *****
      IF(T1)190,190,820
  190 IF(KA-1)195,195,800
C     ***** THE OVERLAPPING ATOM HIDES THE ORIGINAL ATOM *****
  195 ICO=-1
      RETURN
C     ***** STORE OVERLAPPING ATOM *****
  800 ICO=ICO+1
      IF(NCOVER-20)810,805,805
  805 NA=17
      CALL ERROR(ATOMS(1,IA),700)
      NCOVER=NCOVER-1
  810 NCOVER=NCOVER+1
      IJ=1
      DO 815 I=1,3
      DO 815 J=I,3
      COVER(IJ,NCOVER)=QA(I,J,2)
  815 IJ=IJ+1
      NC(NCOVER)=IA
  820 CONTINUE
C     ***** SECOND PART OF SUBROUTINE CHECKS FOR BONDS OVER THE ATOM ***
  825 IF(NQUAD)870,870,830
  830 ITT=0
C     ***** ROUGH CHECK FOR OVERLAPPING BONDS *****
      DO 865 IQ=1,NQUAD
      T10=QUAD(9,IQ)
      NA1=T10/1000.
      NA2=AMOD(T10,1000.)
      IF(NA-NA1)835,835,865
  835 DO 845 J=1,2
      IF(VMAX(J)-AMIN1(QUAD(J,IQ),QUAD(J+2,IQ),QUAD(J+4,IQ),QUAD(J+6,IQ)
     1 ))865,865,840
  840 IF(VMIN(J)-AMAX1(QUAD(J,IQ),QUAD(J+2,IQ),QUAD(J+4,IQ),QUAD(J+6,IQ)
     1 ))845,845,865
  845 CONTINUE
C     ***** EXACT CHECK FOR OVERLAPPING BONDS *****
  850 ITT=ITT+1
      IQQ=IQ
      CALL LAPAB(IQ,NA,IQQ,ITT)
      IF(IQQ)855,860,860
  855 ICO=-1
      RETURN
  860 ICO=ICO+1
      IF(NCOVER-10)865,870,870
  865 CONTINUE
  870 RETURN
      END

      SUBROUTINE LAPBON(NA1,NA2,ICO)
C     ***** SUBROUTINE CHECKS FOR ATOMS AND BONDS OVERLAPPING A BOND ***
      DIMENSION PL(4,4),V1(3),V2(3),VMAX(2),VMIN(2),QUA(3,3)
      DIMENSION VEC(3)
      COMMON/BLAP/CONIC(7,500),COVER(6,20),NC(20),NQ(10),NCONIC,NCOVER,
     1 NCOVQ,NQUAD,NTYPE,QOVER(3,4,10),QUAD(9,400),SPAN(50,2)
      REAL*8 CHPN
      DIMENSION A(9),AA(3,3),AADDV(3,3),AAUDE(3,3),AID(3,3),ATV(10)
      DIMENSION ATOMS(3,500),BO(3,3),CO(3,10),CHIR(100),CONT(5),L(3,110)
      DIMENSION EA(3,3),EP(2,110),EV(3,100),ES(3,3,80),ED(5,10),OPEN(1)
      DIMENSION F(3,100),PA(3,3,100),PAC(3,3),PAT(3,3),QX(3,3),RTPV(3,3)
      DIMENSION RES(80),SHA(5),STND(3,3),TITLE(10),TITLE2(10),T(3,80)
      DIMENSION VP(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),VREF(3,3)
      DIMENSION XLAB(3),XO(3),YP(3)
```

```
      COMMON NT,A,AA,AAOEV,AAUSE,AID,AIU,ATOMS,BD,BBIN,CD,CHIN,CONT,D
      COMMON DD,DP,DISP,FORM,TU,FORT,FS,IU,ITILT,ED,LATB,LTOO,NATOM,NCD
      COMMON NJ,NJJ,NOTT,NW,NSTA,OPOS,P,PQ,PAC,RAT,C,SIGV,SIS,SMS,SCALE
      COMMON SCAL2,SCL,STAR,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2
      COMMON V3,V4,V5,V6,WORD,XLTE,IO,IT
      IJ=0
      ICQ=0
      IF(NA1-NA2)205,205,195
  195 ITEST=FLOAT(NA1)*1000.+FLOAT(NA2)
      IF(NCONIC)205,205,250
  200 IF(NJ2-2)250,235,255
C     ***** PART 1, CALLED FROM BOND, STORES BOND OUTLINE INFORMATION **
  205 IF(NQUAD-500)215,210,210
  210 NN=16
      CALL PRINT(ATOMS(1,NA1),027)
      GO TO 295
  215 NQUAD=NQUAD+1
C     ***** CALCULATE OVERLAP MARGIN FOR BOND QUADRANGLE *****
      T1=0.0
      T2=0.0
      DO 220 J=1,2
      V1(J)=DP(J,1)-DP(J,65)
      V2(J)=DP(J,2)-DP(J,66)
      T1=T1+V1(J)**2
  220 T2=T2+V2(J)**2
      IF(T1*T2)225,225,230
  225 T1=0.0
      T2=0.0
      GO TO 235
  230 T1=OVRMGN/SQRT(T1)
      T2=OVRMGN/SQRT(T2)
C     ***** STORE BOND QUADRANGLE *****
  235 DO 240 J=1,2
      V1(J)=V1(J)*T1
      V2(J)=V2(J)*T2
      QUAD(J,NQUAD)=DP(J,1)+V1(J)
      QUAD(J+2,NQUAD)=DP(J,2)+V2(J)
      QUAD(J+4,NQUAD)=DP(J,66)-V2(J)
  240 QUAD(J+6,NQUAD)=DP(J,65)-V1(J)
      QUAD(9,NQUAD)=ITEST
  245 RETURN
C     ***** PART 2, CALLED FROM BOND, OVERLAP CHECK FOR BOND NA1-NA2 ***
  250 NCOVER=0
      NOVER=0
      TOL=1.E-5
      IF(NCONIC-NA1)285,285,255
C     ***** SAVE QUADRANGLE TEMPORARILY *****
  255 IQ=NQUAD+1
      DO 260 J=1,2
      QUAD(J,IQ)=DP(J,1)
      QUAD(J+2,IQ)=DP(J,2)
      QUAD(J+4,IQ)=DP(J,66)
  260 QUAD(J+6,IQ)=DP(J,65)
      QUAD(9,IQ)=ITEST
C     ***** FIT RECTANGLE AROUND QUADRANGLE *****
  265 DO 270 J=1,2
      VMIN(J)=AMIN1(DP(J,1),DP(J,2),DP(J,66),DP(J,65))
  270 VMAX(J)=AMAX1(DP(J,1),DP(J,2),DP(J,66),DP(J,65))
C     ***** ROUGH CHECK FOR ATOM-OVER-BOND OVERLAP *****
      NA1P1=NA1+1
      IT=0
      DO 285 IA=NA1P1,NCONIC
      DO 285 J=1,2
      IF(IA-NA2)275,285,275
  275 IF(VMAX(J)-CONIC(2*J-1,IA))285,285,280
  280 IF(VMIN(J)-CONIC(2*J,IA))290,285,285
  285 CONTINUE
C     ***** CHECK FOR TRUE ATOM-OVER-BOND OVERLAP *****
      ITT=ITT+1
      CALL LOPAD(IQ,IA,IQQ,ITT)
      IF(IQQ)295,305,300
C     ***** HIDDEN BOND *****
  290 ICQ=-1
  295 RETURN
  300 ICQ=ICQ+1
      IF(NCOVER-20)305,310,310
  305 CONTINUE
  310 IF(NGOOD)295,295,315
C     ***** ROUGH CHECK FOR BOND-OVER-BOND OVERLAP *****
  315 CALL DIFF(ATOMS(2,NA2),ATOMS(2,NA1),V1)
      CALL UNIT(V1,V1,1)
      VN(1)= ATOMS(2,NA1)
      VN(2)= ATOMS(1,NA1)
      VN(3)= ATOMS(4,NA1)-VIEW

      DO 895 ID=1,NQUAD
      T(ID)=QUAD(9,ID)
      IF(ITEST-T(ID))120,895,120
  120 NB2=AMOD(T(ID),1000.)
      NB1=T(ID)/1000.
      IF(NA1-NB2)125,895,895
  125 DO 115 J=1,2
      IF(VMAX(J)-AMIN1(QUAD(J,ID),QUAD(J+2,ID),QUAD(J+4,ID),QUAD(J+6,ID)
     1 ))895,895,110
  110 IF(VMIN(J)-AMAX1(QUAD(J,ID),QUAD(J+2,ID),QUAD(J+4,ID),QUAD(J+6,ID)
     1 ))115,895,895
  115 CONTINUE
C     ***** SET UP LINEAR FORMS FOR EDGES OF QUADRANGLE *****
      DO 145 L=1,4
      K=2*L
      K1=MOD(K,8)+2
      QUA(1,L)=QUAD(K,IQ)-QUAD(K1,IQ)
      QUA(2,L)=QUAD(K1-1,IQ)-QUAD(K-1,IQ)
      QUA(3,L)=QUAD(K-1,IQ)*QUAD(K1,IQ)-QUAD(K,IQ)*QUAD(K1-1,IQ)
C     ***** NORMALIZE LINE EQUATION COEFFICIENTS *****
      T1=SQRT(QUA(1,L)**2+QUA(2,L)**2)
      IF(T1)895,895,140
  140 DO 145 J=1,3
  145 QUA(J,L)=QUA(J,L)/T1
C     ***** EVALUATE LINEAR FORMS AND SIGNATURES FOR QUADRANGLE *****
      T3=1.0
      DO 165 K=1,4
      T2=1.0
      J=2*K
      DO 155 L=1,4
      T1=QUAD(J-1,ID)*QUA(1,L)+QUAD(J,ID)*QUA(2,L)+QUA(3,L)
      IF(T1)150,155,155
  150 T2=T2-1.0
  155 PL(L,K)=T1
      IF(T2)160,165,165
  160 T3=T3-1.0
  165 CONTINUE
C     ***** CHECK FOR 4 POINTS INSIDE QUADRANGLE *****
      IF(T3)170,175,175
  170 ITYPE=-1
      GO TO 915
C     ***** CHECK FOR 1 TO 3 POINTS INSIDE QUADRANGLE ****
  175 IF(T3-4.0)180,185,185
  180 ITYPE=0
      GO TO 915
C     ***** DETERMINE WHICH EDGES ARE CROSSED BY THE 4 LINE SEGMENTS ***
  185 DO 905 L=1,4
      L1=MOD(L,4)+1
C     ***** LINE SEGMENT L FROM POINT V1 TO POINT V2 *****
      V1(1)=QUAD(L*2-1,ID)
      V1(2)=QUAD(L*2,ID)
      V2(1)=QUAD(L1*2-1,ID)
      V2(2)=QUAD(L1*2,ID)
      DO 905 K=1,4
      T1=PL(K,L)
      T2=PL(K,L1)
      T3=T1-T2
C     ***** T1 AND T2 MUST HAVE OPPOSITE SIGNS FOR INTERSECTION TO OCCUR
      IF(T1*T2)190,190,905
C     ***** COMPONENT OF SEGMENT L PERPENDICULAR TO EDGE K OF ID IS T3
  190 IF(ABS(T3)-1.E-5)905,905,195
C     ***** CALCULATE COORDINATES OF INTERSECTION *****
  195 T4=(T1*V2(1)-T2*V1(1))/T3
      T5=(T1*V2(2)-T2*V1(2))/T3
      K0=2*K
      K1=2*(MOD(K,4)+1)
C     ***** IS INTERSECTION WITHIN QUADRANGLE IQ *****
      T6=(T4-QUAD(K0-1,IQ))*(QUAD(K1-1,IQ)-T4)+(T5-QUAD(K0,IQ))*
     1 (QUAD(K1,IQ)-T5)
      IF(ABS(T6)-1.E-5)910,910,900
  900 IF(T6)905,910,910
  905 CONTINUE
      GO TO 895
  910 ITYPE=1
C     ***** CHECK OVER/UNDER AMBIGUITY *****
  915 IF((NA1-NB1)*(NA2-NB2)*(NA2-NB1))925,920,925
C     ***** BONDS SHARE AN ATOM *****
  920 IF(NA1+NA2-NB1-NB2)895,895,895
  925 CALL DIFF(ATOMS(2,NB2),ATOMS(2,NB1),V2)
      CALL DIFF(ATOMS(2,NB1),ATOMS(2,NA1),V3)
      CALL UNIT(V2,V2,1)
      CALL UNIT(V3,V3,1)
      CALL NORM(V1,V2,V4,1)
      IF(VT(V3,V4)-TOL)930,930,935
```

```
C     ***** PARALLEL BONDS, RECALCULATE V3 *****
  830 CALL NORM(V3,V4,V5,1)
      CALL NORM(V5,V1,V3,1)
C     ***** CHECK FOR COLLINEAR BONDS *****
      IF(VV(V3,V3)-TOL)865,865,850
  835 IF(VV(V3,V4)+TCL)840,850,850
  840 DO 845 J=1,3
  845 V3(J)=-V3(J)
C     ***** V3 IS NORMAL TO BONDS IQ AND IB GOING FROM IQ TOWARD IB ***
  850 IF(VIEW)855,855,860
  855 IF(V3(3))895,895,865
  860 IF(VV(ROT,V3))865,895,895
C     ***** OVERLAPPING BOND FOUND *****
  865 ICQ=ICQ+1
      IF(ITYPE)870,875,875
C     ***** HIDDEN BOND *****
  870 ICQ=-1
      RETURN
C     ***** STORE INTERFERING QUADRANGLE *****
  875 IF(NQOVER-30)885,880,880
  880 NG=17
      CALL ERROR(FID2,800)
      RETURN
  885 NQOVER=NQOVER+1
      DO 890 K=1,4
      DO 890 J=1,3
  890 QOVER(J,K,NQOVER)=QUA(J,K)
      NJ(NQOVER)=IB
  895 CONTINUE
  900 RETURN
      END


      SUBROUTINE LAPAB(IQ,IA,ICQ,ITY)
C     ***** SUBROUTINE CHECKS FOR OVERLAP BETWEEN ATOMS AND BONDS *****
C     ***** CALLED BY SUBROUTINES LAP700 AND LAP800 *****
      DIMENSION BP(4),CON(3,3),QP(5),QUA(3,4)
      COMMON/OLAP/CONIC(7,330),COORD(6,20),KC(20),KQ(30),NCONIC,NCOVER,
     1 NQOVER,NQUAD,OVMRGN,QOVER(3,4,30),QUAD(9,600),STOR(50,2)
      REAL*8 CHEM
      DIMENSION A(9),AA(3,3),AAREV(3,3),AANOR(3,3),AID(3,3),AIO(140)
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(164),CONT(5),D(3,130)
      DIMENSION DA(3,3),DP(2,130),EV(3,166),FS(3,3,48),ND(5,10),ORGN(3)
      DIMENSION P(3,166),PA(3,3,166),PAC(3,5),PAT(3,3),Q(3,3),REPV(3,3)
      DIMENSION RES(4),RMS(5),SYMM(3,3),TITLE(10),TITLE2(10),TS(3,48)
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WREV(3,3)
      DIMENSION XLBL(3),XO(3),XT(3)
      COMMON NG,A,AA,AAREV,AANOR,AID,AIN,ATOMS,BB,BBBR,CD,CHEM,CONT,D
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LINC,NATOM,NCD
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REPV,RES,RMS,SCAL1
      COMMON SCAL2,SCL,SYMM,TAPED,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2
      COMMON V3,V4,V5,V6,WREV,XLBL,XO,XT
      TID=QUAD(9,IQ)
      NA1=TID/1000.
      NA2=AMOD(TID,1000.)
C     ***** ITY.GT.0, CHECK FOR ATOMS OVER A BOND ****
C     ***** ITY.LT.0, CHECK FOR BONDS OVER AN ATOM *****
      ICQ=0
      IF(ITY)210,200,205
  200 RETURN
  205 CALL LAPCON(CONIC(1,IA),CON,V1,0.0)
      IF(ITY-2)220,240,240
  210 IF(ITY+2)220,220,215
  215 CALL LAPCON(CONIC(1,IA),CON,V1,OVMRGN)
C     ***** SET UP LINEAR FORMS FOR EDGES OF QUADRANGLE *****
  220 DO 235 L=1,4
      K=2*L
      K1=MOD(K,8)+2
      QUA(1,L)=QUAD(K,IQ)-QUAD(K1,IQ)
      QUA(2,L)=QUAD(K1-1,IQ)-QUAD(K-1,IQ)
      QUA(3,L)=QUAD(K-1,IQ)*QUAD(K1,IQ)-QUAD(K,IQ)*QUAD(K1-1,IQ)
      T1=SQRT(QUA(1,L)**2+QUA(2,L)**2)
      IF(T1)225,225,230
  225 ITY=0
      ICQ=0
      GO TO 430
C     ***** TRANSFORM COEFFICIENTS FOR EDGES TO NORMAL FORM *****
  230 DO 235 J=1,3
  235 QUA(J,L)=QUA(J,L)/T1
C     ***** EVALUATE 4 QUADRATIC AND 4 BILINEAR FORMS *****
  240 V2(3)=1.0
      V3(3)=1.0
      T2=0.0
      DO 265 L=1,4
      L1=(MOD(L,4)+1)*2
      V2(1)=QUAD(2*L-1,IQ)
      V2(2)=QUAD(2*L,IQ)
      V3(1)=QUAD(L1-1,IQ)
      V3(2)=QUAD(L1,IQ)
      QP(L)=0.0
      BP(L)=0.0
      DO 250 K=1,3
      T1=CON(3,K)
      DO 245 J=1,2
  245 T1=T1+V2(J)*CON(J,K)
      QP(L)=QP(L)+T1*V2(K)
  250 BP(L)=BP(L)+T1*V3(K)
      IF(QP(L))260,255,265
  255 T2=T2-0.5
      GO TO 265
  260 T2=T2-1.0
  265 CONTINUE
      QP(5)=QP(1)
C     ***** CHECK FOR 4 POINTS OF QUADRANGLE INSIDE OR ON ELLIPSE *****
      IF(T2)270,275,275
  270 ITYPE=-1
      GO TO 330
C     ***** CHECK FOR 1 TO 3 POINTS OF QUADRANGLE INSIDE THE ELLIPSE ***
  275 IF(T2-2.2)280,285,285
  280 ITYPE=0
      IF(NA2-IA)300,375,335
C     ***** CHECK FOR QUADRANGLE-ELLIPSE INTERSECTION *****
  285 DO 305 K=1,4
C     ***** EVALUATE DISCRIMINANT *****
      T1=BP(K)**2-QP(K)*QP(K+1)
      IF(T1)305,305,290
  290 T1=SQRT(T1)
C     ***** IS INTERSECTION WITHIN BOUNDS OF QUADRANGLE *****
      T3=QP(K)-BP(K)
      T4=T3+QP(K+1)-BP(K)
      IF(ABS(T4)-1.E-5)305,305,295
  295 T5=(T3-T1)/T4
      IF(T5)305,300,300
  300 IF(1.0-T5)305,305,380
  305 CONTINUE
C     ***** NO VALID INTERSECTION FOUND *****
C     ***** CHECK FOR CENTER OF ELLIPSE WITHIN THE QUADRANGLE ****
      T3=1.0
      DO 320 K=1,4
      T1=QUA(3,K)
      DO 310 J=1,2
  310 T1=T1+V1(J)*QUA(J,K)
      IF(T1)315,320,320
  315 T3=T3-1.0
  320 CONTINUE
      IF(T3)325,330,330
  325 ITYPE=1
C     ***** CHECK OVER/UNDER AMBIGUITY *****
  330 IF(NA2-IA)335,375,335
  335 IF(IA-NA1)375,375,340
  340 CALL DIFV(ATOMS(2,NA2),ATOMS(2,NA1),V2)
      CALL DIFV(ATOMS(2,IA),ATOMS(2,NA1),V3)
      CALL UNIT(V2,V2,1)
      CALL UNIT(V3,V3,1)
      CALL NORM(V2,V3,V4,1)
      IF(VV(V4,V4)-1.E-5)345,345,350
C     ***** CENTER OF ATOM IC IS ON THE BOND LINE *****
  345 IF(ITY)370,370,385
C     ***** CENTER OF ATOM IQ IS NOT ON THE BOND LINE *****
  350 CALL NORM(V4,V2,V5,1)
      T1=-V5(3)
      IF(VIEW)365,365,355
  355 T1=V5(3)*(ATOMS(4,IA)-VIEW)
      DO 360 J=1,2
  360 T1=T1+V5(J)*ATOMS(J+1,IA)
  365 IF(T1*FLOAT(ITY))375,375,370
C     ***** NO INTERFERENCE FOUND *****
  370 ICQ=0
      GO TO 410
C     ***** ITYPE=1 ENCLOSED ELLIPSE / ITYPE=-1 ENCLOSED QUADRANGLE ****
  375 IF(ITYPE*ITY)380,385,385
C     ***** HIDDEN ATOM OR HIDDEN BOND *****
  380 ICQ=-1
      GO TO 410
  385 ICQ=1
      IF(ITY)410,390,390
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C     ***** STORE INTERFERING ELLIPSE *****                             LAPA1340
  390 IF(NCOVER-20)400,395,395                                          LAPA1350
  395 NG=17                                                             LAPA1360
      CALL ERPRT(ATOMS(1,IA),800)                                       LAPA1370
      NCOVER=NCOVER-1                                                   LAPA1380
  400 NCOVER=NCOVER+1                                                   LAPA1390
      IJ=1                                                              LAPA1400
      DO 405 I=1,3                                                      LAPA1410
      DO 405 J=I,3                                                      LAPA1420
      COVER(IJ,NCOVER)=CON(I,J)                                         LAPA1430
  405 IJ=IJ+1                                                           LAPA1440
      NC(NCOVER)=IA                                                     LAPA1450
      GO TO 430                                                         LAPA1460
C     ***** STORE INTERFERING QUADRANGLE *****                          LAPA1470
  410 IF(NQOVER-30)420,415,415                                          LAPA1480
  415 NG=19                                                             LAPA1490
      CALL ERPRT(TID,700)                                               LAPA1500
      NQOVER=NQOVER-1                                                   LAPA1510
  420 NQOVER=NQOVER+1                                                   LAPA1520
      DO 425 K=1,4                                                      LAPA1530
      DO 425 J=1,3                                                      LAPA1540
  425 QOVER(J,K,NQOVER)=QUA(J,K)                                        LAPA1550
      NQ(NQOVER)=IQ                                                     LAPA1560
  430 RETURN                                                            LAPA1570
      END                                                               LAPA1580


      SUBROUTINE LAPCON(CON1,CON,T,OVRD)                                LAPC  10
C     ***** TRANSFORM CONIC TO PICTURE HOMOGENEOUS COORDINATE SYSTEM ***LAPC  20
C     ***** CALLED BY SUBROUTINES LAP700 AND LAPAR *****                LAPC  30
      DIMENSION CON1(7),CON(3,3),T(3)                                   LAPC  40
      T(1)=(CON1(1)+CON1(2))*0.5                                        LAPC  50
      T(2)=(CON1(3)+CON1(4))*0.5                                        LAPC  60
      T(3)=1.0                                                          LAPC  70
      CON(1,1)=CON1(5)                                                  LAPC  80
      CON(1,2)=CON1(6)                                                  LAPC  90
      CON(2,1)=CON1(6)                                                  LAPC 100
      CON(2,2)=CON1(7)                                                  LAPC 110
      T1=(CON1(2)-CON1(1)+CON1(4)-CON1(3))*0.25                         LAPC 120
      CON(3,3)=-((T1-OVRD)/T1)**2                                       LAPC 130
      DO 205 K=1,2                                                      LAPC 140
      CON(K,3)=0.0                                                      LAPC 150
      DO 200 J=1,2                                                      LAPC 160
  200 CON(K,3)=CON(K,3)-T(J)*CON(J,K)                                   LAPC 170
      CON(3,K)=CON(K,3)                                                 LAPC 180
  205 CON(3,3)=CON(3,3)-CON(3,K)*T(K)                                   LAPC 190
      RETURN                                                            LAPC 200
      END                                                               LAPC 210


      SUBROUTINE LAPDRW(V,NPEN,NCQ)                                     LAPD  10
C     ***** SUBROUTINE ELIMINATES HIDDEN LINES AND DRAWS VISIBLE LINES *LAPD  20
      DIMENSION CD(20),CQ(50,2),QL(4,30,2),SRQ(2),V(3),VN(3),VO(3),Z(3) LAPD  30
      COMMON/OLAP/CONIC(7,500),COVER(6,20),NC(20),NQ(30),NCONIC,NCOVER, LAPD  40
     1 NQOVER,NQUAD,OVRLAP,QOVER(3,4,30),QUAD(9,600),SEGM(50,2)         LAPD  50
      REAL*8 CHEM                                                       LAPD  60
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    LAPD  70
      DIMENSION ATOMS(4,500),BD(3,3),CD(8,10),CHEM(144),CONT(5),D(3,130)LAPD  80
      DIMENSION DA(3,3),DP(2,130),EV(3,144),FS(3,3,96),KD(5,96),ORGN(3) LAPD  90
      DIMENSION P(3,144),PA(3,3,144),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) LAPD 100
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,96)   LAPD 110
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WORK(3,3)   LAPD 120
      DIMENSION XLNG(3),XO(3),XT(3)                                     LAPD 130
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BD,BRDR,CD,CHEM,CONT,D   LAPD 140
      COMMON DA,DP,DISP,EDGE,EV,FORM,FS,IN,ITILT,KD,LATM,LINE,NATOM,NCD LAPD 150
      COMMON NJ,NJ2,NOUT,NSR,NSTR,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1LAPD 160
      COMMON SCAL2,SCL,SYMB,TAPED,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   LAPD 170
      COMMON V3,V4,V5,V6,WORK,XLNG,XO,XT                                LAPD 180
      NCQ=NCOVER+NQOVER                                                 LAPD 190
      IF(NCQ)200,200,205                                                LAPD 200
  200 RETURN                                                            LAPD 210
C     ***** CHECK ALL OVERLAPPING ATOMS AND BONDS *****                 LAPD 220
  205 NPN3=NPEN-3                                                       LAPD 230
      IF(NPN3)   210,230,230                                            LAPD 240
C     ***** SAVE INFORMATION FROM LAST POINT IF PEN IS DOWN *****       LAPD 250
  210 VO(1)=VN(1)                                                       LAPD 260
      VO(2)=VN(2)                                                       LAPD 270
      VO(3)=1.0                                                         LAPD 280
      NPO=NPN                                                           LAPD 290
      DO 215 K=1,NCQ                                                    LAPD 300
  215 CQ(K,1)=CQ(K,2)                                                   LAPD 310
      IF(NQOVER)230,230,220                                             LAPD 320
  220 DO 225 K=1,NQOVER                                                 LAPD 330
      DO 225 J=1,4                                                      LAPD 340
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  225 QL(J,K,1)=QL(J,K,2)                                               LAPD 350
C     ***** EVALUATE CONIC QUADRATIC FORMS AT NEW POINT VN *****        LAPD 360
  230 VN(1)=V(1)                                                        LAPD 370
      VN(2)=V(2)                                                        LAPD 380
      VN(3)=1.0                                                         LAPD 390
      NPN=NPEN                                                          LAPD 400
      IF(NCOVER)250,250,235                                             LAPD 410
  235 DO 245 K=1,NCOVER                                                 LAPD 420
      Z(1)=VN(1)*COVER(1,K)+VN(2)*COVER(2,K)+COVER(3,K)                 LAPD 430
      Z(2)=VN(1)*COVER(2,K)+VN(2)*COVER(4,K)+COVER(5,K)                 LAPD 440
      Z(3)=VN(1)*COVER(3,K)+VN(2)*COVER(5,K)+COVER(6,K)                 LAPD 450
      CQ(K,2)=Z(1)*VN(1)+Z(2)*VN(2)+Z(3)                                LAPD 460
C     ***** EVALUATE CONIC BILINEAR FORM IF PEN IS DOWN *****           LAPD 470
      IF(NPN3)240,245,245                                               LAPD 480
  240 CD(K)= Z(1)*VO(1)+Z(2)*VO(2)+Z(3)                                 LAPD 490
  245 CONTINUE                                                          LAPD 500
C     ***** EVALUATE LINEAR FORMS AND SIGNATURE FOR QUADRANGLE *****    LAPD 510
  250 IF(NQOVER)275,275,255                                             LAPD 520
  255 NCQ=NCOVER                                                        LAPD 530
      DO 270 K=1,NQOVER                                                 LAPD 540
      T2=3.0                                                            LAPD 550
      DO 265 J=1,4                                                      LAPD 560
      T1=VN(1)*QOVER(1,J,K)+VN(2)*QOVER(2,J,K)+QOVER(3,J,K)             LAPD 570
      IF(T1)260,265,265                                                 LAPD 580
  260 T2=T2-1.0                                                         LAPD 590
  265 QL(J,K,2)=T1                                                      LAPD 600
      NCQ=NCQ+1                                                         LAPD 610
C     ***** T2=-1 INSIDE, +3 ACROSS ANY EDGE, +1 ACROSS ANY VERTEX *****LAPD 620
  270 CQ(NCQ,2)=T2                                                      LAPD 630
C     ***** IF PEN IS UP, OMIT ALL SUBSEQUENT CHECKING *****            LAPD 640
  275 IF(NPN3)285,280,280                                               LAPD 650
  280 NPN=1                                                             LAPD 660
      CALL SCRIBE(VN,NPN,LINE)                                          LAPD 670
      RETURN                                                            LAPD 680
C     ***** CHECK FOR HIDDEN SEGMENT *****                              LAPD 690
  285 DO 295 K=1,NCQ                                                    LAPD 700
      IF(CQ(K,1))290,295,295                                            LAPD 710
  290 IF(CQ(K,2))280,295,295                                            LAPD 720
  295 CONTINUE                                                          LAPD 730
C     ***** FIND ENTRY AND EXIT POINTS OF EACH CONIC *****              LAPD 740
      NINT=0                                                            LAPD 750
      IF(NCOVER)330,330,300                                             LAPD 760
  300 DO 325 K=1,NCOVER                                                 LAPD 770
C     ***** EVALUATE DISCRIMINANT *****                                 LAPD 780
      T1=CD(K)**2-CQ(K,1)*CQ(K,2)                                       LAPD 790
      IF(T1)325,325,305                                                 LAPD 800
  305 T1=SQRT(T1)                                                       LAPD 810
C     ***** SOLVE QUADRATIC EQUATION *****                              LAPD 820
      T2=CQ(K,1)-CD(K)                                                  LAPD 830
      T3=T2+CQ(K,2)-CD(K)                                               LAPD 840
      IF(ABS(T3)-1.E-5)325,325,310                                      LAPD 850
  310 T4=(T2-T1)/T3                                                     LAPD 860
      T5=(T2+T1)/T3                                                     LAPD 870
C     ***** VALID INTERSECTION IF T4.LT.1 AND T5.GT.0 *****             LAPD 880
      IF(T4-1.0)315,325,325                                             LAPD 890
  315 IF(T5)325,325,320                                                 LAPD 900
C     ***** SAVE VALID CONIC INTERSECTIONS *****                        LAPD 910
  320 NINT=NINT+1                                                       LAPD 920
      SEGM(NINT,1)=T4                                                   LAPD 930
      SEGM(NINT,2)=T5                                                   LAPD 940
  325 CONTINUE                                                          LAPD 950
  330 IF(NQOVER)425,425,335                                             LAPD 960
C     ***** FIND ENTRY AND EXIT POINTS FOR EACH QUADRANGLE *****        LAPD 970
  335 DO 420 K=1,NQOVER                                                 LAPD 980
      II2=0                                                             LAPD 990
      NCQ=NCOVER+K                                                      LAPD1000
C     ***** CHECK FOR SINGLE INSIDE POINT *****                         LAPD1010
      SRQ(1)=CQ(NCQ,1)                                                  LAPD1020
      IF(SRQ(1))345,340,340                                             LAPD1030
  340 SRQ(1)=1.0-CQ(NCQ,2)                                              LAPD1040
      IF(SRQ(1)-1.0)350,350,345                                         LAPD1050
C     ***** INSIDE POINT FOUND, ONLY ONE INTERSECTION POSSIBLE *****    LAPD1060
  345 II2=1                                                             LAPD1070
C     ***** FIND WHICH EDGES ARE CROSSED BY THE SEGMENT *****           LAPD1080
  350 DO 410 J=1,4                                                      LAPD1090
      T1=QL(J,K,1)                                                      LAPD1100
      T2=QL(J,K,2)                                                      LAPD1110
      T3=T1-T2                                                          LAPD1120
      IF(T1*T2)355,355,410                                              LAPD1130
C     ***** CHECK FOR SEGMENT ON AN EDGE *****                          LAPD1140
  355 IF(ABS(T3)-1.E-5)420,420,360                                      LAPD1150
C     ***** CALCULATE COORDINATES OF INTERSECTION *****                 LAPD1160
  360 T4=(T1*VN(1)-T2*VO(1))/T3                                         LAPD1170
      T5=(T1*VN(2)-T2*VO(2))/T3                                         LAPD1180
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      J1=2*(MOD(J,4)+1)                                                 LAPD1190
      IQ=NQ(K)                                                          LAPD1200
C     ***** IS INTERSECTION WITHIN LIMITS OF QUADRANGLE *****           LAPD1210
      T6=(T4-QUAD(2*J-1,IQ))*(QUAD(J1-1,IQ)-T4)+(T5-QUAD(2*J,IQ))*      LAPD1220
     1 (QUAD(J1,IQ)-T5)                                                 LAPD1230
      IF(ABS(T6)-1.E-6) 370,370,365                                     LAPD1240
  365 IF(T6)410,370,370                                                 LAPD1250
C     ***** CALCULATE FRACTION PARAMETER AND STORE IT *****             LAPD1260
  370 T1=T1/T3                                                          LAPD1270
      IF(I12-1) 375,380,395                                             LAPD1280
C     ***** STORE FIRST INTERSECTION *****                              LAPD1290
  375 I12=1                                                             LAPD1300
      GO TO 390                                                         LAPD1310
C     ***** STORE SECOND INTERSECTION ****                              LAPD1320
  380 I12=2                                                             LAPD1330
      IF(T1-SEG(1)) 385,405,405                                         LAPD1340
  385 SEG(2)=SEG(1)                                                     LAPD1350
  390 SEG(1)= T1                                                        LAPD1360
      GO TO 410                                                         LAPD1370
C     ***** MORE THAN TWO INTERSECTIONS (I.E.,QUADRANGLE DIAGONAL) *****LAPD1380
  395 IF(T1-SEG(1)) 390,410,400                                         LAPD1390
  400 IF(T1-SEG(2)) 410,410,405                                         LAPD1400
  405 SEG(2)=T1                                                         LAPD1410
  410 CONTINUE                                                          LAPD1420
      IF(I12-1) 420,420,415                                             LAPD1430
C     ***** STORE FRACTION PARAMETERS *****                             LAPD1440
  415 NINT=NINT+1                                                       LAPD1450
      SEGM(NINT,1)=SEG(1)                                               LAPD1460
      SEGM(NINT,2)=SEG(2)                                               LAPD1470
  420 CONTINUE                                                          LAPD1480
C     ***** END OF ENTRY-AND-EXIT-POINT CALCULATIONS *****              LAPD1490
  425 IF(NINT-1) 430,440,435                                            LAPD1500
C     ***** NO INTERFERENCE FOUND, DRAW ENTIRE SEGMENT *****            LAPD1510
  430 CALL SCRIBE(TR,2,LTWO)                                            LAPD1520
      RETURN                                                            LAPD1530
C     **** SORT SEGMENT INTERSECTION LIST *****                         LAPD1540
C     ***** SORTING PROCEDURE BY SHELL,D.L. COMM. ACM 2,30-32 (1959) ***LAPD1550
  435 M=NINT                                                            LAPD1560
  440 M=M/2                                                             LAPD1570
      IF(M) 490,490,445                                                 LAPD1580
  445 K=NINT-M                                                          LAPD1590
      J=1                                                               LAPD1600
  450 I=J                                                               LAPD1610
  455 IM=I+M                                                            LAPD1620
      IF(SEGM(I,1)) 460,470,475                                         LAPD1630
  460 IF(SEGM(IM,1)) 465,465,485                                        LAPD1640
  465 IF(SEGM(I,2)-SEGM(IM,2)) 485,485,475                              LAPD1650
  470 IF(SEGM(I,1)-SEGM(IM,1)) 485,485,475                              LAPD1660
  475 DO 480 L=1,2                                                      LAPD1670
      T1=SEGM(I,L)                                                      LAPD1680
      SEGM(I,L)=SEGM(IM,L)                                              LAPD1690
  480 SEGM(IM,L)=T1                                                     LAPD1700
      I=I-M                                                             LAPD1710
      IF(I) 485,485,455                                                 LAPD1720
  485 J=J+1                                                             LAPD1730
      IF(J-K) 450,450,440                                               LAPD1740
C     ***** FIND STARTING POINT P0 AND END POINT P1 *****               LAPD1750
  490 P0=0.0                                                            LAPD1760
      K=0                                                               LAPD1770
  495 K=K+1                                                             LAPD1780
      IF(K-NINT) 500,500,515                                            LAPD1790
  500 P1=SEGM(K,1)                                                      LAPD1800
      IF(P1) 510,505,505                                                LAPD1810
  505 IF(P1-P0) 510,510,520                                             LAPD1820
  510 P0=AMAX1(P0,SEGM(K,2))                                            LAPD1830
      IF(P0-1.0) 495,525,525                                            LAPD1840
  515 P1=1.0                                                            LAPD1850
C     ***** DRAW SEGMENT FROM P0 TO P1 *****                            LAPD1860
  520 IF(P0) 525,525,530                                                LAPD1870
  525 P0=0.0                                                            LAPD1880
  530 Z(1)=V0(1)*(1.-P0)+VN(1)*P0                                       LAPD1890
      Z(2)=V0(2)*(1.-P0)+VN(2)*P0                                       LAPD1900
      NP=1                                                              LAPD1910
      CALL SCRIBE(Z,NP,LTWO)                                            LAPD1920
      IF(P0-1.0) 535,560,560                                            LAPD1930
  535 Z(1)=V0(1)*(1.-P1)+VN(1)*P1                                       LAPD1940
      Z(2)=V0(2)*(1.-P1)+VN(2)*P1                                       LAPD1950
      NP=2                                                              LAPD1960
      CALL SCRIBE(Z,NP,LTWO)                                            LAPD1970
      IF(P1-1.0) 510,560,560                                            LAPD1980
  560 RETURN                                                            LAPD1990
      END                                                               LAPD2000
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      SUBROUTINE MM(X,Y,Z)                                               MM   10
C     MULTIPLY TWO MATRICES                                              MM   20
C     Z(3,3)=X(3,3)*Y(3,3)                                               MM   30
      DIMENSION X(3,3),Y(3,3),Z(3,3)                                     MM   40
      DO 117 I=1,3                                                       MM   50
      DO 117 K=1,3                                                       MM   60
      Z(I,K)=0.0                                                         MM   70
      DO 117 J=1,3                                                       MM   80
  117 Z(I,K)=Z(I,K)+X(I,J)*Y(J,K)                                        MM   90
      RETURN                                                             MM  100
      END                                                                MM  110


      SUBROUTINE MV(X,Y,Z)                                               MV   10
C     MATRIX * VECTOR                                                    MV   20
C     Z(3)=X(3,3)*Y(3)                                                   MV   30
      DIMENSION X(3,3),Y(3),Z(3)                                         MV   40
      DO 111 I=1,3                                                       MV   50
      Z(I)=0.0                                                           MV   60
      DO 111 J=1,3                                                       MV   70
  111 Z(I)=Z(I)+X(I,J)*Y(J)                                              MV   80
      RETURN                                                             MV   90
      END                                                                MV  100


      SUBROUTINE NORM(X,Y,Z,ITYPE)                                       NORM  10
C     ***** VECTOR PRODUCT  Z=X*Y *****                                  NORM  20
C     ***** ITYPE .GT.0 FOR CARTESIAN,.LE.0 FOR TRICLINIC *****          NORM  30
      DIMENSION X(3),Y(3),Z(3),U1(3)                                     NORM  40
      REAL*8 CHAR                                                        NORM  50
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)     NORM  60
      DIMENSION ATOMS(3,550),BB(3,3),CD(8,10),CNTR(140),CONT(5),D(3,110) NORM  70
      DIMENSION EA(3,3),DP(2,150),EV(3,144),FS(3,3,96),KD(5,15),NG(96)   NORM  80
      DIMENSION P(3,144),PA(3,3,144),PAC(3,3),PAT(3,3),Q(3,3),REFV(3,3)  NORM  90
      DIMENSION RES(40),NRS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,96)   NORM 100
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WORK(3,3)    NORM 110
      DIMENSION XLNG(3),X0(3),XT(3)                                      NORM 120
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHAR,CONT,D    NORM 130
      COMMON DA,DP,DISP,DOLD,EV,FORE,FS,IN,ITILT,KD,LATM,LTYPE,NATOM,NCD NORM 140
      COMMON NJ,NJ2,NOUT,NSR,NSYM,NUMB,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1 NORM 150
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2    NORM 160
      COMMON V3,V4,V5,V6,WORK,XLNG,X0,XT                                 NORM 170
      DO 125 I=1,3                                                       NORM 180
      I1=MOD(I,3)+1                                                      NORM 190
      I2=MOD(I+1,3)+1                                                    NORM 200
      T1=X(I1)*Y(I2)-X(I2)*Y(I1)                                         NORM 210
      IF(ITYPE) 115,115,105                                              NORM 220
  105 Z(I)=T1                                                            NORM 230
      GO TO 125                                                          NORM 240
  115 U1(I)=T1                                                           NORM 250
  125 CONTINUE                                                           NORM 260
      IF(ITYPE) 135,135,140                                              NORM 270
  135 CALL MV(BB,U1,Z)                                                   NORM 280
  140 RETURN                                                             NORM 290
      END                                                                NORM 300


      SUBROUTINE PAXE(AC,DP,ITYPE)                                       PAXE  10
C     ***** ITYPE .LT.0 FOR COVARIANCE MATRIX IN V *****                 PAXE  20
C     ***** ITYPE .GT.0 FOR ELLIPSOID QUADRATIC FORM IN Q *****          PAXE  30
C     ***** IABS(ITYPE)=1 BASED ON TRICLINIC COORDINATE SYSTEM *****     PAXE  40
C     ***** =2 OR 3 FOR WORKING OR REFERENCE CARTESIAN SYSTEMS *****     PAXE  50
C     ***** CONTRAVARIANT EIGENVECTORS PUT IN COLUMNS OF PAC *****       PAXE  60
C     ***** CHECK ATOM CODE *****                                        PAXE  70
      DIMENSION U(3,3),E(3)                                              PAXE  80
      REAL*8 CHAR                                                        PAXE  90
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)     PAXE 100
      DIMENSION ATOMS(3,550),BB(3,3),CD(8,10),CNTR(140),CONT(5),D(3,110) PAXE 110
      DIMENSION EA(3,3),DP(2,150),EV(3,144),FS(3,3,96),KD(5,15),NG(96)   PAXE 120
      DIMENSION P(3,144),PA(3,3,144),PAC(3,3),PAT(3,3),Q(3,3),REFV(3,3)  PAXE 130
      DIMENSION RES(40),NRS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,96)   PAXE 140
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WORK(3,3)    PAXE 150
      DIMENSION XLNG(3),X0(3),XT(3)                                      PAXE 160
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHAR,CONT,D    PAXE 170
      COMMON DA,DP,DISP,DOLD,EV,FORE,FS,IN,ITILT,KD,LATM,LTYPE,NATOM,NCD PAXE 180
      COMMON NJ,NJ2,NOUT,NSR,NSYM,NUMB,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1 PAXE 190
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2    PAXE 200
      COMMON V3,V4,V5,V6,WORK,XLNG,X0,XT                                 PAXE 210
      IP=IABS(ITYPE)-1                                                   PAXE 220
      N3=AMOD(SPCNT,100.)                                                PAXE 230
      IF(N3-NG) 135,115,115                                              PAXE 240
  105 N1=0                                                               PAXE 250
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      GO TO 300                                                         PAXE 260
  115 IT=ACOSZ/190.90,                                                  PAXE 270
      IF(NATOM-IT) 125,130,130                                          PAXE 280
  125 NN=5                                                              PAXE 290
      GO TO 300                                                         PAXE 300
  130 IF(IT) 125,125,135                                                PAXE 310
C     ***** CRYSTALLOGRAPHIC SYMMETRY ROTATION *****                    PAXE 320
  135 CALL TMM(FA(1,1,IT),FS(1,1,NS),PAT)                               PAXE 330
      IF(IT-1) 160,145,155                                              PAXE 340
C     ***** TRANSFORM TO CARTESIAN SYSTEMS *****                        PAXE 350
  145 CALL TMM(PAT,AAUDR,PAC)                                           PAXE 360
      GO TO 175                                                         PAXE 370
  155 CALL TMM(PAT,AAREV,PAC)                                           PAXE 380
      GO TO 175                                                         PAXE 390
  160 IF(ITYPE) 162,175,170                                             PAXE 400
C     ***** TRANSFORM TO TRICLINIC SYSTEM *****                         PAXE 410
  162 DO 165 J=1,9                                                      PAXE 420
  165 PAC(J,1)=PAT(J,1)                                                 PAXE 430
      GO TO 175                                                         PAXE 440
  170 CALL MM(AA,PAT,PAC)                                               PAXE 450
C     ***** FORM DIAGONAL MATRIX OR ITS INVERSE *****                   PAXE 460
  175 DO 205 J=1,3                                                      PAXE 470
      T1=EV(J,II)                                                       PAXE 480
      IF(ITYPE) 195,195,185                                             PAXE 490
  185 Z(J)=1./(T1*T1)                                                   PAXE 500
      GO TO 205                                                         PAXE 510
  195 Z(J)=T1*T1                                                        PAXE 520
  205 PHS(J)=T1                                                         PAXE 530
C     ***** FORM QUADRATIC FORM *****                                   PAXE 540
      DO 265 I=1,3                                                      PAXE 550
      DO 265 J=I,3                                                      PAXE 560
      T1=0.0                                                            PAXE 570
      DO 225 K=1,3                                                      PAXE 580
  225 T1=T1+PAC(I,K)*PAC(J,K)*Z(K)                                      PAXE 590
      Q(J,I)=T1                                                         PAXE 600
  265 Q(I,J)=T1                                                         PAXE 610
  300 RETURN                                                            PAXE 620
      END                                                               PAXE 630

      SUBROUTINE PLTXY(X,Y)                                             PLTX  10
C     ***** PLOT COORD. AND CLOSEST EDGE AFTER PROJECTION *****         PLTX  20
      DIMENSION X(3),Y(2)                                               PLTX  30
      REAL*8 CHEM                                                       PLTX  40
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAUDR(3,3),AID(3,3),AIN(100)    PLTX  50
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(164),CONT(5),D(3,120)PLTX  60
      DIMENSION DA(3,3),DP(2,120),EV(3,164),FS(3,3,96),KD(5,10),NG(2)   PLTX  70
      DIMENSION P(3,164),PA(3,3,164),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) PLTX  80
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,96)   PLTX  90
      DIMENSION V(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)    PLTX 100
      DIMENSION XLMN(4),XO(3),XT(3)                                     PLTX 110
      COMMON NG,A,AA,AAREV,AAUDR,AID,AIN,ATOMS,BB,BBRR,CD,CHEM,CONT,D   PLTX 120
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTDO,NATOM,NCD PLTX 130
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1PLTX 140
      COMMON SCAL2,SCL,SYMB,TAPEB,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   PLTX 150
      COMMON V3,V4,V5,V6,WRKV,XLMN,XO,XT                                PLTX 160
      T0=1.                                                             PLTX 170
      T1=1.                                                             PLTX 180
      IF (VIEW) 125,125,110                                             PLTX 190
  110 T0=VIEW-X(3)                                                      PLTX 200
      IF(T0) 115,115,120                                                PLTX 210
  115 Y(1)=-99.                                                         PLTX 220
      Y(2)=-99.                                                         PLTX 230
      GO TO 130                                                         PLTX 240
  120 T1=VIEW/T0                                                        PLTX 250
  125 Y(1)=X(1)*T1+XO(1)                                                PLTX 260
      Y(2)=X(2)*T1+XO(2)                                                PLTX 270
      T1=XLMN(1)-ABS(Y(1)*2.-XLMN(3))                                   PLTX 280
      T2=XLMN(2)-ABS(Y(2)*2.-XLMN(4))                                   PLTX 290
      EDGE=AMIN1(T1,T2)*.5                                              PLTX 300
      IF(T0-VIEW*0.5) 130,300,300                                       PLTX 310
  130 EDGE=-99.                                                         PLTX 320
  300 RETURN                                                            PLTX 330
      END                                                               PLTX 340

      SUBROUTINE PRELIM                                                 PREL  10
C     ***** DATA INPUT ROUTINE *****                                    PREL  20
      DIMENSION B(9)                                                    PREL  30
      REAL*8 CHEM                                                       PREL  40
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAUDR(3,3),AID(3,3),AIN(100)    PREL  50
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(164),CONT(5),D(3,120)PREL  60
      DIMENSION DA(3,3),DP(2,120),EV(3,164),FS(3,3,96),KD(5,10),NG(2)   PREL  70
      DIMENSION P(3,164),PA(3,3,164),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) PREL  80
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,96)   PREL  90
      DIMENSION V(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)    PREL 100
      DIMENSION XLMN(4),XO(3),XT(3)                                     PREL 110
      COMMON NG,A,AA,AAREV,AAUDR,AID,AIN,ATOMS,BB,BBRR,CD,CHEM,CONT,D   PREL 120
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTDO,NATOM,NCD PREL 130
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1PREL 140
      COMMON SCAL2,SCL,SYMB,TAPEB,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   PREL 150
      COMMON V3,V4,V5,V6,WRKV,XLMN,XO,XT                                PREL 160
C     ***** CELL DIMENSIONS *****                                       PREL 170
  106 FORMAT(6F9.6)                                                     PREL 180
      READ (IN,106) (A(I),I=1,6)                                        PREL 190
      T1=ABS(A(4))-1.                                                   PREL 200
      DO 125 J=1,3                                                      PREL 210
      IF(T1) 115,110,110                                                PREL 220
C     ***** CELL ANGLES IN DEGREES *****                                PREL 230
  110 A(J+6)=A(J+3)                                                     PREL 240
      A(J+3)=COS(A(J+6)*1.7453293E-2)                                   PREL 250
      GO TO 120                                                         PREL 260
C     ***** COSINES OF CELL ANGLES *****                                PREL 270
  115 A(J+6)=ARCCOS(A(J+3))                                             PREL 280
C     ***** STORE IDENTITY MATRIX *****                                 PREL 290
  120 AID(J,J)=1.                                                       PREL 300
      AID(J+1,1)=0.                                                     PREL 310
      AID(J+5,1)=0.                                                     PREL 320
C     ***** STORE METRIC TENSOR *****                                   PREL 330
  125 AA(J,J)=A(J)**2                                                   PREL 340
      AA(1,2)=A(1)*A(2)*A(6)                                            PREL 350
      AA(1,3)=A(1)*A(3)*A(5)                                            PREL 360
      AA(2,3)=A(2)*A(3)*A(4)                                            PREL 370
      AA(2,1)=AA(1,2)                                                   PREL 380
      AA(3,1)=AA(1,3)                                                   PREL 390
      AA(3,2)=AA(2,3)                                                   PREL 400
C     ***** INVERT METRIC TENSOR *****                                  PREL 410
      CALL AINOD(AA,BB,AID,3)                                           PREL 420
C     ***** CALCULATE RECIPROCAL CELL PARAMETERS *****                  PREL 430
      DO 130 J=1,3                                                      PREL 440
  130 B(J)=SQRT(BB(J,J))                                                PREL 450
      B(4)=BB(2,3)/(B(2)*B(3))                                          PREL 460
      B(5)=BB(1,3)/(B(1)*B(3))                                          PREL 470
      B(6)=BB(1,2)/(B(1)*B(2))                                          PREL 480
      DO 138 J=1,3                                                      PREL 490
  138 B(J+6)=ARCCOS(B(J+3))                                             PREL 500
C     ***** WAS INPUT FOR REAL OR RECIPROCAL CELL *****                 PREL 510
      IF(A(4)-1.) 135,150,150                                           PREL 520
  135 DO 140 J=1,9                                                      PREL 530
      T1=AA(J,1)                                                        PREL 540
      AA(J,1)=BB(J,1)                                                   PREL 550
      BB(J,1)=T1                                                        PREL 560
      T1=A(J)                                                           PREL 570
      A(J)=B(J)                                                         PREL 580
  140 B(J)=T1                                                           PREL 590
C     ***** WRITE OUT CELL PARAMETERS *****                             PREL 600
  103 FORMAT(1H0,10X,22HDIRECT CELL PARAMETERS/1H ,14X,1HA,10X,1HB,10X,1HC,10PREL 610
     1X,5HALPHA,6X,4HBETA,5X,5HGAMMA)                                   PREL 620
  105 FORMAT(1H ,9X,F9.4,2F11.4,3F11.3/1H 60X,6HCOSINE,1X,3F11.6)       PREL 630
  107 FORMAT(1H0,10X,26HRECIPROCAL CELL PARAMETERS/1H ,14X,2HA*,11X,2HB*,11XPREL 640
     1,2HC*,11X,6HALPHA*,5X,5HBETA*,6X,6HGAMMA*)                        PREL 650
  150 WRITE (NOUT,103)                                                  PREL 660
      WRITE (NOUT,105) (A(I),I=1,3),(A(I),I=7,9),(A(I),I=4,6)           PREL 670
      WRITE (NOUT,107)                                                  PREL 680
      WRITE (NOUT,105) (B(I),I=1,3),(B(I),I=7,9),(B(I),I=4,6)           PREL 690
C     ***** STORE STANDARD VECTORS *****                                PREL 700
      CALL AIRE(AID,AID(1,2),REFV,0)                                    PREL 710
      CALL MM(AA,REFV,AAREV)                                            PREL 720
      DO 160 I=1,3                                                      PREL 730
      DO 160 J=1,3                                                      PREL 740
      AAUDR(J,I)=AAREV(J,I)                                             PREL 750
      Q(J,I)=REFV(I,J)                                                  PREL 760
  160 WRKV(J,I)=REFV(J,I)                                               PREL 770
C     ***** READ AND WRITE SYMMETRY TRANSFORMATIONS *****               PREL 780
  171 FORMAT(1H0,10X,24HSYMMETRY TRANSFORMATIONS/1H 10X,3HNO.,12X,11HTRANSLATIOPREL 790
     1N,8X,10HX TRANSFORMED ,10X,11HY TRANSFORMED 8X)                   PREL 800
  173 FORMAT(I1,F14.10,3F1.0,2(F15.10,3F3.0))                           PREL 810
  175 FORMAT(1H 11X,I2,3(F13.6,F6.0,2H X,F6.0,2H Y,F6.0,2H Z))          PREL 820
  177 FORMAT(1H1,10X,18A4)                                              PREL 830
      WRITE (NOUT,171)                                                  PREL 840
      LINES=10                                                          PREL 850
      DO 190 I=1,96                                                     PREL 860
      LINES=MOD(LINES+1,56)                                             PREL 870
      READ (IN,173) IS,(TS(J,I),(FS(K,J,I),K=1,3),J=1,3)                PREL 880
      IF (LINES) 185,180,185                                            PREL 890
  180 WRITE (NOUT,177) (TITLE(J),J=1,18)                                PREL 900
      WRITE (NOUT,171)                                                  PREL 910
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  105 WRITE (NOUT,175)I,(TS(J,1),(TS(K,J,1),K=1,3),J=1,4)               PREL 920
C     ***** NON-CRYSTALLOGRAPHIC HELIX-SYMMETRY INPUT *****              PREL 930
      IF(TS(1,3,I)-5.)100,106,106                                        PREL 940
  106 T1=TS(1,3,I)/TS(3,3,I)                                             PREL 950
      TS(3,I)=TS(3,I)*T1                                                 PREL 960
      T1=AMOD(T1*TS(2,3,I),1.)*6.28318531)                               PREL 970
      T2=COS(T1)                                                         PREL 980
      T1=SIN(T1)                                                         PREL 990
      DO 107 J=1,9                                                       PREL1000
  107 VT(J,1)=AID(J,1)                                                   PREL1010
      VT(1,1)=T2                                                         PREL1020
      VT(2,2)=T2                                                         PREL1030
      VT(2,1)=-T1                                                        PREL1040
      VT(1,2)=T1                                                         PREL1050
      CALL MM(VT,Q,PAC)                                                  PREL1060
      CALL MM(AAWRT,PAC,TS(1,1,I))                                       PREL1070
  100 IF(IS)105,190,105                                                  PREL1080
  190 CONTINUE                                                           PREL1090
      NI=1                                                               PREL1100
      CALL ERPNT(0.,0)                                                   PREL1110
      I=N4                                                               PREL1120
  195 NSYM=I                                                             PREL1130
C     ***** POSITIONAL AND THERMAL PARAMETERS *****                      PREL1140
  207 FORMAT(11H0NO.  ATOM 12,1H5I0X,1H6I0X,1H5I1X,1H8I10X,1H92X8,1H031PREL1150
     10X,1H51207,1H3110X,1H0921    TYPE)                                 PREL1160
  209 FORMAT(1H 13,1X,A6,3F11.6,5X,6F11.6,F5.0)                          PREL1170
  210 FORMAT(1H 13,1X,A6,1F11.6,5X,2F11.0,0F11.0,F5.0)                   PREL1180
  211 FORMAT(A6,3X,5F9.0,F9.0)                                           PREL1190
  213 FORMAT(I3,F9.6,5F9.0,7X,F2.0)                                      PREL1200
      LINES=LINES+2                                                      PREL1210
      IF(LINES-54)220,215,215                                            PREL1220
  215 LINES=-1                                                           PREL1230
      GO TO 225                                                          PREL1240
  220 WRITE (NOUT,207)                                                   PREL1250
  225 DO 265 I=1,164                                                     PREL1260
      LINES=MOD(LINES+1,54)                                              PREL1270
      READ (IN,211)CHEM(I),V1(1),V1(2),(P(J,I),J=1,3),V1                 PREL1280
      K=1.+V1                                                            PREL1290
      IF(FLOAT(K-1)-V1)227,228,227                                       PREL1300
  227 K=1                                                                PREL1310
  228 READ (IN,213)IS,(PA(J,1,I),J=1,7)                                  PREL1320
      IF(LINES)230,230,232                                               PREL1330
  230 WRITE (NOUT,177)(TITLE(J),J=1,18)                                  PREL1340
      WRITE (NOUT,207)                                                   PREL1350
  232 IF(PA(1,1,I)-10000.)235,236,236                                    PREL1360
  236 WRITE (NOUT,210)I,CHEM(I),(P(J,I),J=1,3),(PA(J,1,I),J=1           PREL1370
     1,7)                                                                PREL1380
      GO TO 238                                                          PREL1390
  235 WRITE (NOUT,209)I,CHEM(I),(P(J,I),J=1,3),(PA(J,1,I),J=1           PREL1400
     1,7)                                                                PREL1410
  238 GO TO (240,239,261,262,240),K                                      PREL1420
C     ***** TYPE 1 POSITIONAL PARAMETERS (ANGSTROMS) *****               PREL1430
  239 DO 240 J=1,3                                                       PREL1440
  240 P(J,I)=P(J,I)/A(J)                                                 PREL1450
      GO TO 264                                                          PREL1460
C     ***** TYPE 2 POSITIONAL PARAMETERS, STANDARD CARTESIAN *****       PREL1470
  261 V1(1)=P(1,I)                                                       PREL1480
      V1(2)=P(2,I)                                                       PREL1490
      GO TO 263                                                          PREL1500
C     ***** TYPE 3 POSITIONAL PARAMETERS *****                           PREL1510
C     ***** CYLINDRICAL COORDINATES REFERRED TO STANDARD CARTESIAN *****PREL1520
  262 T2=P(2,I)*.01745329252                                             PREL1530
      V1(1)=V1(1)+P(1,I)*COS(T2)                                         PREL1540
      V1(2)=V1(2)+P(1,I)*SIN(T2)                                         PREL1550
  263 V1(3)=P(3,I)                                                       PREL1560
      CALL MV(V1,Q,P(1,I))                                               PREL1570
  264 IF(IS)266,265,266                                                  PREL1580
  265 CONTINUE                                                           PREL1590
      NI=2                                                               PREL1600
      CALL ERPNT(0.,0)                                                   PREL1610
      I=120                                                              PREL1620
  266 NATOM=I                                                            PREL1630
C     ***** CONVERT TEMP FACTOR COEF TO STANDARD TYPE ZERO *****         PREL1640
      NI=3                                                               PREL1650
      DO 450 I=1,NATOM                                                   PREL1660
      T1=PA(1,1,I)                                                       PREL1670
      K=1.+PA(7,1,I)                                                     PREL1680
      IF(T1)250,250,255                                                  PREL1690
  250 T1=.1                                                              PREL1700
      GO TO 605                                                          PREL1710
  255 T6=.0506605918                                                     PREL1720
      GO TO(270,260,265,265,270,260,600,605,270,260,270,450),K           PREL1730
C     ***** TYPE 1 *****                                                 PREL1740
  260 DO 262 J=4,6                                                       PREL1750
  262 PA(J,1,I)=PA(J,1,I)*.5                                             PREL1760
      GO TO 270                                                          PREL1770
C     ***** TYPES 2 AND 3 (BASE 2 SYSTEMS) *****                         PREL1780
  265 T6=.1515152066                                                     PREL1790
      IF(K-4)270,260,270                                                 PREL1800
C     ***** TYPES 0 THROUGH 5 *****                                      PREL1810
  270 IF(PA(7,1,I))600,600,272                                           PREL1820
  272 DO 300 J=1,3                                                       PREL1830
      DO 300 L=J,3                                                       PREL1840
      T2=T6                                                              PREL1850
      IF(K-5)285,275,275                                                 PREL1860
  275 IF(K-6)280,280,281                                                 PREL1870
C     ***** TYPES 4 AND 5 *****                                          PREL1880
  280 T2=B(J)*B(L)*T2*.25                                                PREL1890
      GO TO 285                                                          PREL1900
C     ***** TYPES 8 AND 9 (B(I,J) TENSOR SYSTEMS) *****                  PREL1910
  281 T2=B(J)*B(L)                                                       PREL1920
      IF(K-11)285,282,282                                                PREL1930
C     ***** TYPE 10, (CARTESIAN TENSOR SYSTEM) *****                     PREL1940
  282 T2=1.0                                                             PREL1950
  285 IF(J-L)290,287,290                                                 PREL1960
  287 VT(J,J)=T2*PA(J,1,I)                                               PREL1970
      GO TO 300                                                          PREL1980
  290 M=J+L+1                                                            PREL1990
      VT(J,L)=T2*PA(M,1,I)                                               PREL2000
      VT(L,J)=VT(J,L)                                                    PREL2010
  300 CONTINUE                                                           PREL2020
C     ***** FIND PRINCIPAL AXES *****                                    PREL2030
      IF(K-11)310,305,305                                                PREL2040
  305 CALL MM(VT,Q,PAC)                                                  PREL2050
      CALL MM(QINV,PAC,VT)                                               PREL2060
  310 CALL MM(VT,AA,DA)                                                  PREL2070
      CALL EIGEN(DA,DRS,PAT)                                             PREL2080
C     ***** ARE EIGENVALUES POSITIVE *****                               PREL2090
      IF(DRS(1))325,325,320                                              PREL2100
  320 IF(NG)350,340,330                                                  PREL2110
  325 NG=1                                                               PREL2120
  330 NG=NI                                                              PREL2130
      CALL ERPNT(FLOAT(I)+19000./.15501.,0)                              PREL2140
C     ***** 3 EQUAL EIGENVALUES, USE REFERENCE VECTORS *****             PREL2150
  340 T1=SIGN(SQRT(ABS(DRS(1)+DRS(2)+DRS(3))/3.),DRS(1))                PREL2160
      DO 345 J=1,3                                                       PREL2170
      DO 342 K=1,6                                                       PREL2180
  342 PA(J,K,I)=REFV(J,K)                                                PREL2190
  345 VV(J,I)=T1                                                         PREL2200
      GO TO 450                                                          PREL2210
  350 IF(NG+4)360,360,352                                                PREL2220
C     ***** TWO EQUAL EIGENVALUES *****                                  PREL2230
  352 M=NG+5                                                             PREL2240
      CALL UNIT(PAT(1,M),V1,-1)                                          PREL2250
      DO 356 K=1,3                                                       PREL2260
      IF(ABS(VMV(V1,AA,REFV(1,K)))-.50)354,356,356                       PREL2270
  354 CONTINUE                                                           PREL2280
  356 CALL MM(AA,DA,VT)                                                  PREL2290
      CALL AXES(V1,REFV(1,K),DA,-1)                                      PREL2300
      DO 359 K=1,3                                                       PREL2310
      L=MOD(M+K+2,3)+1                                                   PREL2320
      DO 358 J=1,3                                                       PREL2330
  358 PA(J,L,I)=DA(J,K)                                                  PREL2340
  359 VV(L,I)=SIGN(SQRT(ABS(VMV(DA(1,K),VT,DA(1,K)))),DRS(L))            PREL2350
      GO TO 450                                                          PREL2360
C     ***** UNIT EIGENVECTORS 1 ANGSTROM LONG *****                      PREL2370
  360 CALL AXES(PAT(1,1),PAT(1,2),PA(1,1,I),-1)                          PREL2380
  370 NG=1                                                               PREL2390
C     ***** ROOT EIGENVALUE = RMS DISPLACEMENT *****                     PREL2400
      DO 375 J=1,3                                                       PREL2410
      T2=DRS(J)                                                          PREL2420
  375 VV(J,I)=SIGN(SQRT(ABS(T2)),T2)                                     PREL2430
      GO TO 450                                                          PREL2440
C     ***** TYPE 6 (ISOTROPIC TEMP FACTOR) *****                         PREL2450
  600 T1=SQRT(T1*1.266515E-2)                                            PREL2460
C     ***** TYPE 7 (DUMMY SPHERE) *****                                  PREL2470
  605 DO 610 J=1,3                                                       PREL2480
  610 VV(J,I)=T1                                                         PREL2490
      IF(PA(1,1,I))610,610,615                                           PREL2500
C     ***** DEFINES VECTORS FOR SPHERE *****                             PREL2510
  615 DO 625 J=1,6                                                       PREL2520
      T2=PA(J+3,1,I)                                                     PREL2530
      CALL ATOM(T2,VT(1,J))                                              PREL2540
      IF(NG)620,625,620                                                  PREL2550
  620 CALL ERPNT(T2,0)                                                   PREL2560
      GO TO 610                                                          PREL2570
  625 CONTINUE                                                           PREL2580
      CALL DIFV(VT(1,2),VT(1,1),V1)                                      PREL2590
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      CALL DIFV(VT(1,4),VT(1,3),V3)                                     PRFL2600
      CALL NORM(V1,V2,PA(1,1,I),-1)                                     PRFL2610
      GO TO 650                                                         PRFL2620
C     ***** DIRECT VECTORS FOR SPHERE *****                             PRFL2630
  635 DO 645 J=1,3                                                      PRFL2640
  645 PA(J,1,I)=UNIT(J,1)                                               PRFL2650
  650 NI=2                                                              PRFL2660
C     ***** WRITE OUT THE VALUES *****                                  PRFL2670
      LINES=LINES+2                                                     PRFL2680
      IF(LINES-56)660,660,655                                           PRFL2690
  655 LINES=-1                                                          PRFL2700
      GO TO 660                                                         PRFL2710
  656 WRITE (NOUT,651)                                                  PRFL2720
  660 DO 665 I=1,NATOM                                                  PRFL2730
      LINES=MOD(LINES+1,56)                                             PRFL2740
      IF (LINES) 665,662,665                                            PRFL2750
  661 FORMAT(1H0ATOM, 6X4H ATOM 42,1HX 10X,1HY 10X,1HZ 11X,7HCOSIN 1 42,7HCOSIN 2 4PRFL2760
     1X,7HCOSIN 3 )                                                     PRFL2770
  662 WRITE (NOUT,771) (TITLE(J),J=1,10)                                PRFL2780
      WRITE (NOUT,661)                                                  PRFL2790
  663 FORMAT(1H I3,1X,A4,3F11.4)                                        PRFL2800
  665 WRITE (NOUT,209) I,CHEM(I),(P(J,I),J=1,3),(TV(J,I),J=1,3          PRFL2810
     1)                                                                 PRFL2820
      IF (NT1)999,999,670                                               PRFL2830
  670 CALL EXIT                                                         PRFL2840
  999 RETURN                                                            PRFL2850
      END                                                               PRFL2860


      SUBROUTINE PRIMO                                                  PRIM  10
C     *****GENERAL INITIALIZATION OF PRIME PARAMETERS*****              PRIM  20
      REAL*8 CHEM                                                       PRIM  30
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(150)    PRIM  40
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(166),CONT(5),D(3,110)PRIM  50
      DIMENSION DA(3,3),DP(2,110),EV(3,166),FS(3,3,80),ID(5,10),ORGN(3) PRIM  60
      DIMENSION P(3,166),PA(3,3,166),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) PRIM  70
      DIMENSION RES(8),RMS(5),SYMM(3,3),TITLE(10),TITLE2(10),TS(3,48)   PRIM  80
      DIMENSION VT(3,8),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   PRIM  90
      DIMENSION XLNG(3),XO(3),XT(3)                                     PRIM 100
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   PRIM 110
      COMMON DA,DP,DISP,FORE,EV,FORM,FS,ID,ITILT,ND,LATM,LTMC,NATOM,NCD PRIM 120
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1PRIM 130
      COMMON SCAL2,SCL,SYMM,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   PRIM 140
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                PRIM 150
      BRDR=0.5                                                          PRIM 160
C     *****CALCULATE CONSTANTS*****                                     PRIM 170
      DO 2999 I=1,5                                                     PRIM 180
 2999 CONT(I)=SQRT(1./(2.*(1.-COS(3.14159)   /2.**I))))                 PRIM 190
      DISP=.005                                                         PRIM 200
      FORE=.066                                                         PRIM 210
      IN=5                                                              PRIM 220
      ITILT=0                                                           PRIM 230
      LATM=0                                                            PRIM 240
      NCD=0                                                             PRIM 250
      NG=0                                                              PRIM 260
      NOUT=6                                                            PRIM 270
      NSR=0                                                             PRIM 280
      RES(1)=1.25                                                       PRIM 290
      RES(2)=.5                                                         PRIM 300
      RES(3)=.2                                                         PRIM 310
      SCAL1=1.0                                                         PRIM 320
      SCAL2=1.50                                                        PRIM 330
      SCL=1.50                                                          PRIM 340
      DO 1000 I=1,3                                                     PRIM 350
      SYMM(I,I)=1.                                                      PRIM 360
      SYMM(I+1,I)=0.                                                    PRIM 370
 1000 SYMM(I+5,I)=0.                                                    PRIM 380
      TAPER=.375                                                        PRIM 390
      THETA=0.0                                                         PRIM 400
      VIEW=0.0                                                          PRIM 410
      XLNG(1)=17.0                                                      PRIM 420
      XLNG(2)=11.0                                                      PRIM 430
      XO(1)=0.5                                                         PRIM 440
      XO(2)=0.5                                                         PRIM 450
      DO 1001 J=1,3                                                     PRIM 460
 1001 ORGN(J) = 0.0                                                     PRIM 470
C     ***** INITIATE OVERLAP ROUTINES *****                             PRIM 480
      CALL LAP500(0)                                                    PRIM 490
      RETURN                                                            PRIM 500
      END                                                               PRIM 510


      SUBROUTINE PROJ(D,DP,E,EO,VIEW,I1,I2,I3)                          PROJ  10
C     ***** 3D CARTESIAN TO 2D PLOTTER COORDINATES *****                PROJ  20
      DIMENSION D(3,129),DP(2,129),E(3),EO(3)                           PROJ  30
      T1=VIEW-E(3)                                                      PROJ  40
      DO 165 I=I1,I2,I3                                                 PROJ  50
      T1=D(1,I)-E(1)                                                    PROJ  60
      T2=D(2,I)-E(2)                                                    PROJ  70
      IF(VIEW) 115,115,120                                              PROJ  80
  120 T3=VIEW/(T1-D(3,I))                                               PROJ  90
      T1=T1*T3                                                          PROJ 100
      T2=T2*T3                                                          PROJ 110
  115 DP(1,I)=T1+EO(1)                                                  PROJ 120
  165 DP(2,I)=T2+EO(2)                                                  PROJ 130
      RETURN                                                            PROJ 140
      END                                                               PROJ 150


      SUBROUTINE RADIAL(ND)                                             RADI  10
C     ***** GENERATE ELLIPSE FROM TWO CONJUGATE VECTORS *****           RADI  20
C     ***** ORTHOGONAL VECTORS PRODUCE A 128 SPACED CIRCLE *****        RADI  30
C     ***** ND DENOTES NUMBER OF SUBDIVISIONS (1 TO 5) *****            RADI  40
      REAL*8 CHEM                                                       RADI  50
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(150)    RADI  60
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(166),CONT(5),D(3,110)RADI  70
      DIMENSION DA(3,3),DP(2,110),EV(3,166),FS(3,3,80),ID(5,10),ORGN(3) RADI  80
      DIMENSION P(3,166),PA(3,3,166),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) RADI  90
      DIMENSION RES(8),RMS(5),SYMM(3,3),TITLE(10),TITLE2(10),TS(3,48)   RADI 100
      DIMENSION VT(3,8),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   RADI 110
      DIMENSION XLNG(3),XO(3),XT(3)                                     RADI 120
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   RADI 130
      COMMON DA,DP,DISP,FORE,EV,FORM,FS,ID,ITILT,ND,LATM,LTMC,NATOM,NCD RADI 140
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1RADI 150
      COMMON SCAL2,SCL,SYMM,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   RADI 160
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                RADI 170
      DO 115 J=1,3                                                      RADI 180
      T1=DA(J,1)                                                        RADI 190
      D(J,1)=T1                                                         RADI 200
      D(J,129)=T1                                                       RADI 210
      D(J,65)=-T1                                                       RADI 220
      T1=DA(J,2)                                                        RADI 230
      D(J,33)=T1                                                        RADI 240
  115 D(J,97)=-T1                                                       RADI 250
      DO 135 N=1,ND                                                     RADI 260
      T1=CONT(N)                                                        RADI 270
      KDEL=2**(6-N)                                                     RADI 280
      KDEL1=KDEL+1                                                      RADI 290
      KDEL2=KDEL/2                                                      RADI 300
      DO 135 L=KDEL1,65,KDEL                                            RADI 310
      J=L-KDEL                                                          RADI 320
      K=L-KDEL2                                                         RADI 330
      DO 135 M=1,3                                                      RADI 340
      T2=(D(M,L)+D(M,J))*T1                                             RADI 350
      D(M,K)=T2                                                         RADI 360
  135 D(M,K+64)=-T2                                                     RADI 370
      RETURN                                                            RADI 380
      END                                                               RADI 390


      SUBROUTINE SCRIBE(V,NPEN,LTYP)                                    SCRI  10
      DIMENSION V(2),VO(2)                                              SCRI  20
C     ***** SUBROUTINE WHICH LINKS WITH THE PLOTTER-SPECIFIC SUBROUTINESSCRI  30
      IF(NPEN-1) 210,205,205                                            SCRI  40
C     ***** KEEP TRACK OF COORDINATES FOR LAST PEN-UP LOCATION *****    SCRI  50
  205 VO(1)=V(1)                                                        SCRI  60
      VO(2)=V(2)                                                        SCRI  70
      NPO=0                                                             SCRI  80
      RETURN                                                            SCRI  90
  210 IF(LTYP) 230,205,215                                              SCRI 100
C     ***** CALL MECHANICAL PLOTTER PLOTTING SUBROUTINE *****           SCRI 110
  215 IF(NPO) 225,220,225                                               SCRI 120
  220 CALL PLOT(VO(1),VO(2),3)                                          SCRI 130
  225 CALL PLOT(V(1),V(2),2)                                            SCRI 140
      GO TO 245                                                         SCRI 150
C     ***** CALL CRT PLOTTING SUBROUTINE *****                          SCRI 160
  230 IF(NPO) 240,235,240                                               SCRI 170
  235 CALL CRT(VO(1),VO(2),0,1)                                         SCRI 180
  240 CALL CRT(V(1),V(2),-LTYP,1)                                       SCRI 190
  245 NPO=1                                                             SCRI 200
      RETURN                                                            SCRI 210
      END                                                               SCRI 220


      SUBROUTINE SHADE                                                  SHAD  10
      DIMENSION NS(8),DX(3),E(2,200),G(3),P(3),Q(2,8),UU(2,3),X(4),Y(3) SHAD  20
      DIMENSION Z(5)                                                    SHAD  30
      REAL*8 CHEM                                                       SHAD  40
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      DIMENSION A(3),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    SEAD  50
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(144),CONT(5),D(3,110)SEAD  60
      DIMENSION DA(3,3),DP(2,110),EV(3,144),FS(3,3,96),KD(5,10),NG(1)   SEAD  70
      DIMENSION P(3,144),PA(3,3,144),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) SEAD  80
      DIMENSION RES(40),RMS(5),SYMB(3,3),TITLE(10),TITLE2(10),TS(3,96)  SEAD  90
      DIMENSION V7(3,6),V1(6),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   SEAD 100
      DIMENSION XLMN(3),XO(3),XT(3)                                     SEAD 110
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   SEAD 120
      COMMON DA,DP,DISP,EDGE,EV,FORM,FS,IN,ITILT,KD,LATM,LTMC,MATOM,NFO SEAD 130
      COMMON NJ,NJ2,NOUT,NSR,NSYM,NORM,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1SEAD 140
      COMMON SCAL2,SCL,SYMB,TAPED,THETA,TITLE,TITLE2,TS,VIEW,V7,V1,V2   SEAD 150
      COMMON V3,V4,V5,V6,WRKV,XLMN,XO,XT                                SEAD 160
C     ***** OBTAIN PROBLEM PARAMETERS *****                             SEAD 170
      WRITE (NOUT,20)                                                   SEAD 180
   20 FORMAT(1H0 9X,62H         FROM ATOMS     TO ATOMS      WITH RADIUS ORSEAD 190
     1, IF A ROW, WITH SYMMETRY[illegible] /11X,[illegible]   (MIN  MAX)    (MIN SEAD 200
     2 MAX)               78,1HA 1,1HMAX,1HC)                           SEAD 210
      IF(AIN(1)-10000.)100,100,101                                      SEAD 220
  100 ITOM1=AIN(1)                                                      SEAD 230
      SYTOM1=55501.                                                     SEAD 240
      GO TO 102                                                         SEAD 250
  101 ITOM1=AIN(1)/100000.                                              SEAD 260
      SYTOM1=AMOD(AIN(1),100000.)                                       SEAD 270
  102 IF(ABS(AIN(2))-10000.)103,103,104                                 SEAD 280
  103 ITOM2 = ABS(AIN(2))                                               SEAD 290
      SYTOM2=SYTOM1                                                     SEAD 300
      GO TO 105                                                         SEAD 310
  104 ITOM2=ABS(AIN(2))/100000.                                         SEAD 320
      SYTOM2=AMOD(ABS(AIN(2)),100000.)                                  SEAD 330
  105 ITAB1=AIN(3)                                                      SEAD 340
      IF(ITAB1)108,108,110                                              SEAD 350
  108 ITAB1=1                                                           SEAD 360
  110 ITAB2=AIN(4)                                                      SEAD 370
      DMAX=AIN(5)                                                       SEAD 380
      IF(DMAX)115,115,120                                               SEAD 390
  115 DMAX=4.                                                           SEAD 400
      AIN(5)=DMAX                                                       SEAD 410
  120 DMX=DMAX*DMAX                                                     SEAD 420
      TEMP=.01                                                          SEAD 430
      NNNN=NJ2*1000+MOD(NJ2,10)                                         SEAD 440
      N=NJ2*100+NJ2                                                     SEAD 450
      IO=SYTOM1                                                         SEAD 460
      IOJ=SYTOM2                                                        SEAD 470
      LATOM=LATM                                                        SEAD 480
  121 FORMAT(1H0 I0X,2I7,I5,I4,I5,2I6,I8,3F9.3/1H )                     SEAD 490
      WRITE (NOUT,121)N,ITOM1,IO,ITOM2,IO2,                             SEAD 500
     1ITAB1,ITAB2,(AIN(J),J=5,7)                                        SEAD 510
  124 FORMAT(1H  I5X,2I5,I4,I5,2F9.3)                                   SEAD 520
      IF(NCD)130,130,125                                                SEAD 530
  125 WRITE (NOUT,124) ((KD(J,I),J=1,4),(CD(J,I),J=1,2) ,I=1,           SEAD 540
     1NCD)                                                              SEAD 550
  130 DO 135 J=1,6                                                      SEAD 560
      W(1,J)=99.                                                        SEAD 570
  135 W(2,J)=-99.                                                       SEAD 580
      DO 155 I=ITAB1,ITAB2                                              SEAD 590
      T1=FLOAT(I)*100000.                                               SEAD 600
      CALL ATOM(T1,X)                                                   SEAD 610
      IF(NG)143,145,143                                                 SEAD 620
  143 CALL PRPRT(T1,ERRR)                                               SEAD 630
      GO TO 600                                                         SEAD 640
  145 X(4)=X(1)-X(2)                                                    SEAD 650
      DO 155 J=1,6                                                      SEAD 660
      TEM=X(J)                                                          SEAD 670
      IF(W(2,J)-TEM)144,152,152                                         SEAD 680
  144 W(2,J)=TEM                                                        SEAD 690
  152 IF(TEM-W(1,J))153,155,155                                         SEAD 700
  153 W(1,J)=TEM                                                        SEAD 710
  155 CONTINUE                                                          SEAD 720
      NNNN2=MOD(NNNN,10)                                                SEAD 730
      GO TO (160,165,160,155,165,165),NNNN2                             SEAD 740
C     ***** FIND PARALLELEPIPEDS WHICH ENCLOSES TRICLINIC ONE *****     SEAD 750
  156 DO 158 J=1,3                                                      SEAD 760
  158 XT(J)=AIN(J+5)                                                    SEAD 770
      GO TO 172                                                         SEAD 780
C     ***** FIND PARALLELEPIPEDS WHICH ENCLOSES ORTHOGONAL ONE *****    SEAD 790
  160 DO 162 I=1,3                                                      SEAD 800
      XT(I)=0.                                                          SEAD 810
      DO 162 J=1,3                                                      SEAD 820
  162 XT(I)=XT(I)+ABS(AAREV(J,I))*DISTAN(J))                            SEAD 830
      GO TO 170                                                         SEAD 840
C     ***** FIND PARALLELEPIPED WHICH ENCLOSES SMALL SPHERE *****       SEAD 850
  165 [illegible]                                                       SEAD 860
      DO 166 J=1,3                                                      SEAD 870
  166 XT(J)=SQRT(([illegible])/[illegible])                             SEAD 880
C     ***** START SEARCH AROUND REFERENCE ATOMS *****                   SEAD 890
  170 LIST=0                                                            SEAD 900
      LAST=0                                                            SEAD 910
      N1=ITOM1                                                          SEAD 920
      N1=ITOM2                                                          SEAD 930
      IF(NUM2-5)186,172,172                                             SEAD 940
C     ***** CONVOLUTE AND ALTERNATIVE CONVOLUTE INSTRUCTIONS *****      SEAD 950
  172 IF(LATM)174,174,176                                               SEAD 960
C     ***** FAULT, NO ENTRIES IN  ATOM LIST *****                       SEAD 970
  174 NG=12                                                             SEAD 980
      CALL PRPRT(0.,ERRR)                                               SEAD 990
      GO TO 600                                                         SEAD1000
C     ***** CHECK FOR REFERENCE ATOMS IN ATOMS LIST *****               SEAD1010
  176 IF(LATM-LAST)600,600,177                                          SEAD1020
  177 LIST=LAST                                                         SEAD1030
      LAST=LATM                                                         SEAD1040
  178 LIST=LIST+1                                                       SEAD1050
      IF(LAST-LIST)505,180,180                                          SEAD1060
  180 T1=ATOMS(1,LIST)                                                  SEAD1070
      ITOM=T1/100000.                                                   SEAD1080
      IF(ITOM-ITOM1)178,182,182                                         SEAD1090
  182 IF(ITOM2-ITOM)178,184,184                                         SEAD1100
  184 SYTOM=AMOD(T1,100000.)                                            SEAD1110
      SYTOM2=SYTOM                                                      SEAD1120
      N1=ITOM                                                           SEAD1130
      N1=ITOM                                                           SEAD1140
C     ***** SET INITIAL RUN PARAMETERS *****                            SEAD1150
  186 N2=AMOD(SYTOM1,100.)                                              SEAD1160
      N5=AMOD(SYTOM1/100.,1000.)                                        SEAD1170
      N3=N5/100                                                         SEAD1180
      N4=MOD(N5/10,10)                                                  SEAD1190
      N5=MOD(N5,10)                                                     SEAD1200
C     ***** SET TERMINAL RUN PARAMETERS *****                           SEAD1210
      M2=AMOD(SYTOM2,100.)                                              SEAD1220
      M5=AMOD(SYTOM2/100.,1000.)                                        SEAD1230
      M3=M5/100                                                         SEAD1240
      M4=MOD(M5/10,10)                                                  SEAD1250
      M5=MOD(M5,10)                                                     SEAD1260
C     ***** START SEARCH AROUND REFERENCE ATOMS *****                   SEAD1270
      DO 500 L5=N5,M5                                                   SEAD1280
      DO 500 L4=N4,M4                                                   SEAD1290
      DO 500 L3=N3,M3                                                   SEAD1300
      DO 500 L2=N2,M2                                                   SEAD1310
      DO 500 ITOM=N1,M1                                                 SEAD1320
      T1=FLOAT(ITOM)*100000.+FLOAT(L3*10000+L4*1000+L5*100+L2)          SEAD1330
      CALL ATOM(T1,Y)                                                   SEAD1340
      IF(NG)188,190,188                                                 SEAD1350
  188 CALL PRPRT(T1,ERRR)                                               SEAD1360
      GO TO 500                                                         SEAD1370
C     ***** F-SYMMETRY EQUIVALENT POSITION *****                        SEAD1380
  190 NU=0                                                              SEAD1390
      DO 400 K=1,NSYM                                                   SEAD1400
C     ***** SUBTRACT SYMMETRY TRANSLATION FROM REFERENCE ATOM *****     SEAD1410
      DO 192 J=1,3                                                      SEAD1420
  192 V1(J)=Y(J)-TS(J,K)                                                SEAD1430
C     ***** DETERMINE LIMITING CELLS TO BE SEARCHED *****               SEAD1440
C     ***** FIRST,MOVE THE DOT THROUGH THE SYMMETRY OPERATION *****     SEAD1450
      DO 200 I=1,3                                                      SEAD1460
      DO 200 L=1,2                                                      SEAD1470
      WW(L,I)=0.0                                                       SEAD1480
      DO 200 J=1,3                                                      SEAD1490
      TEM=FS(I,J,K)                                                     SEAD1500
      IF(TEM)194,200,196                                                SEAD1510
  194 M=MOD(L,2)+1                                                      SEAD1520
      GO TO 198                                                         SEAD1530
  196 M=L                                                               SEAD1540
  198 WW(L,I)=WW(L,I)+W(M,J)*TEM                                        SEAD1550
  200 CONTINUE                                                          SEAD1560
C     ***** CHECK FOR RIGHT INPUT TRANSFORMATION *****                  SEAD1570
      DO 211 I=1,3                                                      SEAD1580
      TEM=FS(I,J,K)                                                     SEAD1590
      IF(NNNN2-(2*J+K))209,211,210                                      SEAD1600
  209 IF(TEM)203,211,207                                                SEAD1610
  203 WW(1,J)=-W(2,K)*TEM                                               SEAD1620
      WW(2,J)=-W(1,K)*TEM                                               SEAD1630
      GO TO 211                                                         SEAD1640
  207 WW(1,J)=W(1,K)*TEM                                                SEAD1650
      WW(2,J)=W(2,K)*TEM                                                SEAD1660
  211 CONTINUE                                                          SEAD1670
C     ***** MOVE A CELLS EDGE THEN MOVE BACK UNTIL PARALLELEPIPED BE WORKSEAD1680
C         [illegible] AND [illegible] TRANSFORMED ATOM [illegible] ***** SEAD1690
      N=0                                                               SEAD1700
      DO 215 J=1,3                                                      SEAD1710
      DO 215 I=1,2                                                      SEAD1720
      N=N+1                                                             SEAD1730
      TE=[illegible](WW(I,J)+V1(J)[illegible])+D1(J)                    SEAD1740
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      TEMP=5.0                                                            SPAR1750
  221 TEMP=TEMP-1.0                                                       SPAR1760
      IF(TEMP)225,225,221                                                 SPAR1770
  225 NU(M)=TEMP+FLOAT(IT2-1)*5.                                          SPAR1780
C     ***** IF NO POSSIBILITY OF A HIT, GO TO NEXT SYMMETRY CARD *****    SPAR1790
      IF(NU(M)-NU(M-1))230,235,235                                        SPAR1800
  235 CONTINUE                                                            SPAR1810
      LL=NU(1)                                                            SPAR1820
      LU=NU(2)                                                            SPAR1830
      ML=NU(3)                                                            SPAR1840
      MU=NU(4)                                                            SPAR1850
      NL=NU(5)                                                            SPAR1860
      NU=NU(6)                                                            SPAR1870
C     ***** L CELL TRANSLATIONS IN X *****                                SPAR1880
      DO 195 L=LL,LU                                                      SPAR1890
      T(1)=U(1)+FLOAT(L-5)                                                SPAR1900
C     ***** M CELL TRANSLATIONS IN Y *****                                SPAR1910
      DO 195 M=ML,MU                                                      SPAR1920
      T(2)=U(2)+FLOAT(M-5)                                                SPAR1930
C     ***** N CELL TRANSLATIONS IN Z *****                                SPAR1940
      DO 195 NN=NL,NU                                                     SPAR1950
      T(3)=U(3)+FLOAT(NN-5)                                               SPAR1960
C     ***** I = TARGET ATOM *****                                         SPAR1970
      DO 195 I=ITAR1,ITAR2                                                SPAR1980
      DO 250 J=1,3                                                        SPAR1990
      TEMP=0.                                                             SPAR2000
      DO 245 K=1,3                                                        SPAR2010
  245 TEMP=TEMP+(X(I,K)-T(K))*G(K,J)                                      SPAR2020
C     ***** SEE IF WITHIN PARALLELEPIPED*****                             SPAR2030
      TEMP=TEMP-V(J)                                                      SPAR2040
      IF(DV(J)-ABS(TEMP))195,250,250                                      SPAR2050
  250 VT(J)=TEMP                                                          SPAR2060
      GO TO (255,255,252,255,255,255),KPNAT                               SPAR2070
C     ***** SEE IF WITHIN SHELL ONE *****                                 SPAR2080
  252 CALL DOT(VT,ADOTV,VT(3))                                            SPAR2090
      DO 253 J=2,3                                                        SPAR2100
      IF(ATOM(J+1)-ABS(VT(J)))195,253,253                                 SPAR2110
  253 CONTINUE                                                            SPAR2120
      GO TO 277                                                           SPAR2130
C     ***** SEE IF WITHIN SPHERE *****                                    SPAR2140
  255 DSQ=DOTS(VT,AA,VT)                                                  SPAR2150
      IF(DMX-DSQ)195,256,256                                              SPAR2160
  256 IF(DSQ-.0001)258,260,261                                            SPAR2170
  258 IF(MOVE-2)195,260,260                                               SPAR2180
  260 TEMP=SQRT(DSQ)                                                      SPAR2190
      IF(ATM(I))265,265,261                                               SPAR2200
C     *****SELECT ONLY ATOM IN ASYMMETRIC UNIT IF REQUESTED *****         SPAR2210
  261 IF(LS-M)265,265,262                                                 SPAR2220
  262 ITEST=FLOAT(I)*100000.                                              SPAR2230
      ITEST=ITEST+TEMP*1000.                                              SPAR2240
      DO 264 J=1,LAST                                                     SPAR2250
      ITEMP=ATOMS(1,J)                                                    SPAR2260
      IF(ITEST-ITEMP)264,263,264                                          SPAR2270
  263 IF(MOVE-ITEM)264,264,195                                            SPAR2280
  264 CONTINUE                                                            SPAR2290
C     ***** SELECT VECTORS ACCORDING TO CODES IF ANY *****                SPAR2300
  265 IF(NCD)277,277,266                                                  SPAR2310
  266 DO 275 J=1,NCD                                                      SPAR2320
  269 IF(ITMP-ICD(1,J))275,270,270                                        SPAR2330
  270 IF(ICD(2,J)-ITMP)275,271,271                                        SPAR2340
  271 IF(I-CD(3,J))    275,272,272                                        SPAR2350
  272 IF(CD(4,J)-I)    275,273,273                                        SPAR2360
  273 IF(TEMP-CD(5,J)) 275,274,274                                        SPAR2370
  274 IF(CD(6,J)-TEMP) 275,277,277                                        SPAR2380
  275 CONTINUE                                                            SPAR2390
      GO TO 195                                                           SPAR2400
  277 T1(1) = 100000.*FLOAT(I)+FLOAT(((1110-L*100-M*10-NN)*1000+K))       SPAR2410
      IF(MOVE-2)278,125,125                                               SPAR2420
C     ***** DETERMINE CORRECT POSITION IN SORTED VECTOR TABLE *****       SPAR2430
  278 IF(NUM)117,117,279                                                  SPAR2440
  279 DO 285 II=1,NUM                                                     SPAR2450
      TT=S(2,II)-TEM                                                      SPAR2460
      IF(ABS(TT)-.0001)281,282,283                                        SPAR2470
  281 IF(TT)115,282,283                                                   SPAR2480
C     ***** MOVE LONGER VECTORS TOWARD END OF TABLE *****                 SPAR2490
  283 IF(300-NUM)287,287,288                                              SPAR2500
  287 NUM=299                                                             SPAR2510
  288 IJ=NUM                                                              SPAR2520
      DO 289 J=II,NUM                                                     SPAR2530
      S(1,IJ+1)=S(1,IJ)                                                   SPAR2540
      S(2,IJ+1)=S(2,IJ)                                                   SPAR2550
  289 IJ=IJ-1                                                             SPAR2560
      GO TO 119                                                           SPAR2570
C     ***** CHECK FOR DUPLICATE VECTORS IF DISTANCES ARE EQUAL *****      SPAR2580
  282 CALL ATOM(S(1,II),R)                                                SPAR2590
      DO 105 J=1,3                                                        SPAR2600
      IF(ABS(U(J)+T(J)-R(J))-0.5000)105,105,115                           SPAR2610
  105 CONTINUE                                                            SPAR2620
      GO TO 195                                                           SPAR2630
  115 CONTINUE                                                            SPAR2640
      IF(300-NUM)120,120,117                                              SPAR2650
C     ***** STORE THE VECTOR IN VECTOR TABLE *****                        SPAR2660
  117 NUM=NUM+1                                                           SPAR2670
  119 NII=NUM+1                                                           SPAR2680
      S(1,II)=T1(1)                                                       SPAR2690
      S(2,II)=TEM                                                         SPAR2700
  120 IF(MOVE-1)195,125,125                                               SPAR2710
C     ***** STORE PRIMED IN ATOMS TABLE *****                             SPAR2720
  125 DO 130 J=1,3                                                        SPAR2730
  130 [illegible]                                                         SPAR2740
      CALL STOP                                                           SPAR2750
  195 CONTINUE                                                            SPAR2760
  405 CONTINUE                                                            SPAR2770
C     ***** PRINT OUT DISTANCES *****                                     SPAR2780
  421 FORMAT(1H0,10X,26HDISTANCES FROM ATOM   (I3,I4,I5,I6)= F,8H10 ATOM TO,SPAR2790
     118H [illegible]                                                     SPAR2800
      IO = [illegible]                                                    SPAR2810
      WRITE (NOUT,421)ITOM,IC,ITAR1,ITAR2                                 SPAR2820
      IF(NUM)500,500,421                                                  SPAR2830
  421 DO 418 I=1,NUM                                                      SPAR2840
      T2=S(1,I)                                                           SPAR2850
      I1=T2/100000.                                                       SPAR2860
      T2=T2-FLOAT(I1)*100000.                                             SPAR2870
      CALL ATOM(T2,R)                                                     SPAR2880
      IF(I-1)412,412,413                                                  SPAR2890
  423 FORMAT(1H ,I3,2(A6,I3),[illegible]                                  SPAR2900
  424 FORMAT(1H ,I3,2(A6,I3),[illegible]                                  SPAR2910
  412 WRITE (NOUT,423)CHEM(ITOM),CHEM(I1),ITOM,I1,(T(J),J=1,3),           SPAR2920
     1I1,I2,I3,[illegible]                                                SPAR2930
      GO TO 418                                                           SPAR2940
  413 WRITE (NOUT,424)CHEM(ITOM),CHEM(I1),I1,I2,(T(J),J=1,3),             SPAR2950
     1S(2,I))                                                             SPAR2960
  418 CONTINUE                                                            SPAR2970
C     ***** CALCULATE ANGLES ABOUT REF ATOM IF CONT IS 1OR2 *****         SPAR2980
  417 IF(MOVE-1)500,451,500                                               SPAR2990
  441 FORMAT(1H0,10X,38HBOND ANGLES ABOUT ATOM(S))                        SPAR3000
  451 WRITE (NOUT,441)ITOM                                                SPAR3010
      L=NUM-1                                                             SPAR3020
      IF(L)500,500,453                                                    SPAR3030
  453 DO 485 I=1,L                                                        SPAR3040
      T2=S(1,I)                                                           SPAR3050
      T3=S(2,I)                                                           SPAR3060
      I1=T2/100000.                                                       SPAR3070
      I2=T2-FLOAT(I1)*100000.                                             SPAR3080
      CALL ATOM(T2,R)                                                     SPAR3090
      CALL DIFF(R,T,W)                                                    SPAR3100
      CALL DOTS(W,G,W2)                                                   SPAR3110
      M=I+1                                                               SPAR3120
      DO 485 J=M,NUM                                                      SPAR3130
      T0=S(1,J)                                                           SPAR3140
      J1=T0/100000.                                                       SPAR3150
      J2=T0-FLOAT(J1)*100000.                                             SPAR3160
      CALL ATOM(T0,R)                                                     SPAR3170
      CALL DIFF(R,T,V)                                                    SPAR3180
      Z=ARCCOS(DOTS(W,G,V)/(TEMS(2,J)))                                   SPAR3190
      CALL DOTS(V,G,V1)                                                   SPAR3200
      Z=[illegible]                                                       SPAR3210
  480 FORMAT(1H ,I3,[illegible] (I3,I4,I5,I6),[illegible]                 SPAR3220
     1 [illegible])                                                       SPAR3230
  485 WRITE (NOUT,480)CHEM(I1),CHEM(ITOM),CHEM(J1),I1,I2,ITOM             SPAR3240
     1,I0,J1,J2,T3,Z                                                      SPAR3250
  485 CONTINUE                                                            SPAR3260
  500 CONTINUE                                                            SPAR3270
      IF(LAST-LIST)505,505,170                                            SPAR3280
  505 IF(NUMSYM-1)600,170,600                                             SPAR3290
  600 IF(MOVE-1)610,605,610                                               SPAR3300
  605 LAST=LATOM                                                          SPAR3310
  610 RETURN                                                              SPAR3320
      END                                                                 SPAR3330

      SUBROUTINE SPAR(INST)                                               SPAR  10
C     ***** INSTRUCTION 1231 PRODUCES PUNCHED CARDS WITH POSIT,(THERMAL   SPAR  20
C     ***** PARAMETERS FOR ATOMS PLACED IN THE ATOMS LIST BY THE ADD      SPAR  30
C     ***** SPECIAL INSTRUCTIONS                                          SPAR  40
      REAL*8 CHEM                                                         SPAR  50
      DIMENSION A(9),AA(3,3),AAINV(3,3),AAVEC(3,3),AIN(3,3),ATM(500)      SPAR  60
      DIMENSION ATOMS(8,500),BB(3,3),CD(6,10),CHEM(500),CODE(5),D(3,110)  SPAR  70
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      DIMENSION DA(3,3),DP(2,150),FF(3,165),FS(3,3,96),KD(5,10),ORGN(3)
      DIMENSION P(3,165),PA(3,3,165),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3)
      DIMENSION RES(8),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,96)
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)
      DIMENSION XLNG(3),XO(3),XT(3)
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D
      COMMON DA,DP,DISP,EDGE,FF,FORT,FS,IN,ITILT,KD,LATM,LTEST,NATOM,NCD
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT
      REAL*8 CHM
C     ***** FIRST FIELD OF INSTRUCTION CARD = NO. OF POSITION PARAMETER
C     ***** CARDS TO BE READ BY THIS SUBROUTINE (STANDARD CARD3 FORMAT)
C     ***** THE SEQUENCE OF THESE CARDS NEED NOT BE IDENTICAL WITH
C     ***** THE ORIGINAL INPUT ATOM DECK SEQUENCE
      IF(ITEST-1201) 100,105,100
  100 NG = 5
      RETURN
  105 IF(AIN(1)) 100,100,115
  115 LAST = AIN(1)
      DO 150 L=1,LAST
      READ (IN,116) CHN,V2(1),V2(2),(V1(J),J=1,6)
  116 FORMAT(A6,3X,6F9.6)
      WRITE (NOUT,117) CHN,V2(1),V2(2),(V1(J),J=1,6)
  117 FORMAT(1H0,20X,25HOLD POSITION PARAMETERS  ,A6,A2,6F10.6)
C     ***** FIND ATOM NUMBER *****
      DO 125 IA=1,NATOM
      DO 120 J=1,3
      IF(ABS(V1(J)-P(J,IA))-0.001) 120,120,125
  120 CONTINUE
      IT = IA
      GO TO 130
  125 CONTINUE
      GO TO 150
C     ***** SEARCH ATOMS LIST FOR ENTRIES WITH ATOM NUMBER IT *****
  130 IF(LATM) 150,150,131
  131 DO 145 IB=1,LATM
      T1 = ATOMS(4,IB)
      IF(IT-INT(T1/100000.)) 145,135,145
  135 CALL ATOM(T1,V1)
      WRITE (NOUT,136) T1,CHN,V2(1),V2(2),(V1(J),J=1,6)
  136 FORMAT(1H0,9X,F10.0,9X,25HNEW POSITION PARAMETERS  ,A6,A2,6F10.6)
      I1 = T1
      PUNCH 137, CHN,V2(1),V2(2),(V1(J),J=1,6),I1
  137 FORMAT(A6,3X,6F9.6,9X,I9)
      CALL PAXES(T1,-1)
      DO 140 I=1,3
      DO 140 J=1,3
  140 Q(J,I) = Q(J,I) /.0506605918
      WRITE (NOUT,141) Q(1,1),Q(2,2),Q(3,3),Q(1,2),Q(1,3),Q(2,3)
  141 FORMAT(1H ,26X,25HNEW THERMAL PARAMETERS   ,6F10.6)
      PUNCH 142, Q(1,1),Q(2,2),Q(3,3),Q(1,2),Q(1,3),Q(2,3),I1
  142 FORMAT(6F9.6,18X,I9)
  145 CONTINUE
  150 CONTINUE
  300 RETURN
      END


      SUBROUTINE STOR
C     ***** STORE IN OR REMOVE FROM ATOMS ARRAY *****
      REAL*8 CHEM
      DIMENSION A(3),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(165),CONT(5),D(3,130)
      DIMENSION DA(3,3),DP(2,150),FF(3,165),FS(3,3,96),KD(5,10),ORGN(3)
      DIMENSION P(3,165),PA(3,3,165),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3)
      DIMENSION RES(8),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,96)
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)
      DIMENSION XLNG(3),XO(3),XT(3)
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D
      COMMON DA,DP,DISP,EDGE,FF,FORT,FS,IN,ITILT,KD,LATM,LTEST,NATOM,NCD
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT
      IF(LATM) 881,881,450
  450 IF(500-LATM) 455,455,460
  455 IF(NJ2-10) 890,890,460
  460 L=LATM
C     ***** CHECK FOR POSITIONAL DUPLICATION *****
      DO 880 N=1,L
      DO 865 J=1,4
      IF(ABS(V1(J)-ATOMS(J,N))-0.001) 865,865,880
  865 CONTINUE
      IF(NJ2-10) 890,890,870
C     ***** ATOM REMOVAL BY TABLE SHORTENING *****
  870 LATM=LATM-1
      DO 875 I=N,LATM
      DO 875 J=1,4
  875 ATOMS(J,I)=ATOMS(J,I+1)
      GO TO 890
  880 CONTINUE
  881 IF(NJ2-10) 882,890,890
C     ***** STORE ATOM *****
  882 IF(499-LATM) 883,883,885
  883 NG=16
      CALL PRINT (V1(1),800)
  885 LATM=LATM+1
      DO 886 J=1,4
  886 ATOMS(J,LATM)=V1(J)
  890 RETURN
      END


      SUBROUTINE TRM(X,Y,Z)
C     ***** TRANSPOSE(TRANSPOSE(X)*Y)=Z *****
C     ***** X,Y,Z ARE 3X3 MATRICES *****
      DIMENSION X(3,3),Y(3,3),Z(3,3)
      DO 115 I=1,3
      DO 115 K=1,3
  115 Z(K,I)=X(1,I)*Y(1,K)+X(2,I)*Y(2,K)+X(3,I)*Y(3,K)
      RETURN
      END


      SUBROUTINE UNITY(X,Z,ITYPE)
      DIMENSION X(3),Y(3),Z(3)
      REAL*8 CHEM
      DIMENSION A(3),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(165),CONT(5),D(3,130)
      DIMENSION DA(3,3),DP(2,150),FF(3,165),FS(3,3,96),KD(5,10),ORGN(3)
      DIMENSION P(3,165),PA(3,3,165),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3)
      DIMENSION RES(8),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,96)
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)
      DIMENSION XLNG(3),XO(3),XT(3)
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D
      COMMON DA,DP,DISP,EDGE,FF,FORT,FS,IN,ITILT,KD,LATM,LTEST,NATOM,NCD
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT
      Y(1)=X(1)
      Y(2)=X(2)
      Y(3)=X(3)
      IF (ITYPE) 125,125,105
  105 T1=SQRT(Y(1)*Y(1)+Y(2)*Y(2)+Y(3)*Y(3))
      GO TO 165
  125 T1=SQRT(Y(1)*(Y(1)*AA(1,1)+Y(2)*(AA(1,2)+AA(2,1))+Y(3)*(AA(1,3)+
     1AA(3,1)))+Y(2)*(Y(2)*AA(2,2)+Y(3)*(AA(2,3)+AA(3,2)))+Y(3)*Y(3)*AA(
     23,3))
  165 IF (T1) 155,155,175
  155 NG=5
      GO TO 300
  175 Z(1)=Y(1)/T1
      Z(2)=Y(2)/T1
      Z(3)=Y(3)/T1
  300 RETURN
      END


      SUBROUTINE VM(X,Y,Z)
C     TRANSPOSED VECTOR TIMES MATRIX
C     Z(J)=X(I)*Y(I,J)
      DIMENSION X(3),Y(3,3),Z(3)
      DO 115 J=1,3
      Z(J)=0.0
      DO 115 I=1,3
  115 Z(J)=Z(J)+X(I)*Y(I,J)
      RETURN
      END


      FUNCTION VMV(X1,Q,X2)
C     TRANSPOSED VECTOR * MATRIX * VECTOR
C     VMV=X1(I)*Q(I,J)*X2(J)      TO  EVALUATE QUADRATIC OR BILINEAR FORM
      DIMENSION X1(3),Q(3,3),X2(3)
      T1=0.
      DO 10 J=1,3
   10 T1=T1+X1(J)*(X2(1)*Q(J,1)+X2(2)*Q(J,2)+X2(3)*Q(J,3))
      VMV=T1
```

```
      RETURN                                                            VMV   90
      END                                                               VMV  100

      FUNCTION VV(X,Y)                                                  VV    10
C     TRANSPOSED VECTOR * VECTOR                                        VV    20
C     VV=X(I)*Y(I)                                                      VV    30
      DIMENSION X(3),Y(3)                                               VV    40
      VV=X(1)*Y(1)+X(2)*Y(2)+X(3)*Y(3)                                  VV    50
      RETURN                                                            VV    60
      END                                                               VV    70

      SUBROUTINE XYZ(QA,X,ITYPE)                                        XYZ   10
C     ***** ITYPE .GT.0 CART. COORD. FROM ATOM CODE WORD *****          XYZ   20
C     ***** IABS(ITYPE) .LE.2 FOR WORKING SYSTEM *****                  XYZ   30
C     ***** IABS(ITYPE) .GT.2 FOR REFERENCE SYSTEM *****                XYZ   40
C     ***** ITYPE .LE.0 USES TRICLINIC COORD. XT *****                  XYZ   50
      DIMENSION X(3)                                                    XYZ   60
      REAL*8 CHEM                                                       XYZ   70
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    XYZ   80
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(500),CONT(5),D(3,120)XYZ   90
      DIMENSION DA(3,3),DP(2,120),EV(3,500),FS(3,3,96),NG(5,10),ORGN(3) XYZ  100
      DIMENSION P(3,500),PA(3,3,500),PAC(3,5),PAT(3,3),Q(3,3),QTEM(3,3) XYZ  110
      DIMENSION RMS(96),RES(5),SYMB(3,3),TITLE(10),TITLE2(10),TS(3,96)  XYZ  120
      DIMENSION VT(3,8),V1(3),V2(3),V3(3),V4(3),V5(3),V6(3),UNIT(3,3)   XYZ  130
      DIMENSION XLNG(3),XO(3),XT(3)                                     XYZ  140
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   XYZ  150
      COMMON DA,DP,DISP,DMAX,EV,FORM,FS,IN,ITILT,KD,LATM,LTYP,NATOM,NCD XYZ  160
      COMMON NJ,NJ2,NOUT,NSR,NSTA,ORGN,P,PA,PAC,PAT,Q,QTEMP,RES,RMS,SCAL1XYZ  170
      COMMON SCAL2,SCL,SYMB,TAPED,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   XYZ  180
      COMMON V3,V4,V5,V6,UNIT,XLNG,XO,XT                                XYZ  190
      IT=IABS(ITYPE)-2                                                  XYZ  200
      NG1=NG                                                            XYZ  210
      NG=0                                                              XYZ  220
      IF(ITYPE) 10,10,5                                                 XYZ  230
    5 CALL ATOM(QA,XT)                                                  XYZ  240
      IF(NG) 30,10,30                                                   XYZ  250
   10 T1=0.                                                             XYZ  260
      DO 15 J=1,3                                                       XYZ  270
      T2=XT(J)-ORGN(J)                                                  XYZ  280
      V1(J)=T2                                                          XYZ  290
   15 T1=T1+ABS(T2)                                                     XYZ  300
      IF(T1-.0001) 20,20,40                                             XYZ  310
   20 NG=NG1                                                            XYZ  320
   30 DO 35 J=1,3                                                       XYZ  330
   35 X(J)=0.                                                           XYZ  340
      GO TO 100                                                         XYZ  350
   40 IF(IT) 45,45,60                                                   XYZ  360
C     ***** RELATIVE TO WORKING SYSTEM *****                            XYZ  370
   45 DO 55 I=1,3                                                       XYZ  380
      T1=0.                                                             XYZ  390
      DO 50 J=1,3                                                       XYZ  400
   50 T1=T1+V1(J)*AAWRK(J,I)                                            XYZ  410
   55 X(I)=T1*SCAL1                                                     XYZ  420
      GO TO 100                                                         XYZ  430
C     ***** RELATIVE TO REFERENCE SYSTEM *****                          XYZ  440
   60 DO 70 I=1,3                                                       XYZ  450
      T1=0.                                                             XYZ  460
      DO 65 J=1,3                                                       XYZ  470
   65 T1=T1+V1(J)*AAREV(J,I)                                            XYZ  480
   70 X(I)=T1*SCAL1                                                     XYZ  490
  100 RETURN                                                            XYZ  500
      END                                                               XYZ  510

      SUBROUTINE CPT(X1,Y1,X2,Y2)                                       CPT   10
C     ***** DUMMY SUBROUTINE TO REPLACE THE CATHODE-RAY-TUBE PACKAGE ***CPT   20
C     ***** SUBROUTINE CPT IS CALLED BY SUBROUTINES F200 AND F810 ***** CPT   30
      RETURN                                                            CPT   40
      END                                                               CPT   50

      SUBROUTINE IDAT(ND)                                               IDAT  10
C     ***** DUMMY FOR ORNL LOCAL SUBROUTINE CALLED BY F200 FOR CPT INPUTIDAT  20
C     ***** IDAT OBTAINS DATE (8 BCD CHARACTERS) FROM OPERATING SYSTEM  IDAT  30
      RETURN                                                            IDAT  40
      END                                                               IDAT  50
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      SUBROUTINE JOBNO(NJ)                                              JOBN  10
C     ***** DUMMY FOR ORNL LOCAL SUBROUTINE CALLED BY F200 FOR CPT INPUTJOBN  20
C     ***** JOBNO OBTAINS ORNL JOB NUMBER (8 BCD CHARACTERS) *****      JOBN  30
      RETURN                                                            JOBN  40
      END                                                               JOBN  50

 CUBANE  E.B.FLEISCHER   1964  J.A.C.S.  86,3889                        STER  10
     5.20      5.20      5.20     72.26     72.26     72.26             STER  20
          0  1  0  0          0  0  1  0          0  0  0  1            STER  30
          0  0  0  1          0  1  0  0          0  0  1  0            STER  40
          0  0  1  0          0  0  0  1          0  1  0  0            STER  50
          0 -1  0  0          0  0 -1  0          0  0  0 -1            STER  60
          0  0  0 -1          0 -1  0  0          0  0 -1  0            STER  70
1         0  0 -1  0          0  0  0 -1          0 -1  0  0            STER  80
 C1                           -.10711    .15519    .10706      0        STER  90
   .00100    .00290    .00500 -.00020   -.01020   -.00510      0        STER 100
 C2                            .11900    .11900    .11900      0        STER 110
   .00400    .00400    .00400 -.01030   -.01030   -.01030      0        STER 120
 H1                           -.17000    .10000    .10000      0        STER 130
      .10                                                      7        STER 140
 H2                            .21000    .21000    .21000      0        STER 150
      .10                                                      7        STER 160
 DUMY                               0         0         0      0        STER 170
1                                                              0        STER 180
    1   101  155501          2         1         0      1.61            STER 190
***** FIND ALL NEIGHBOR ATOMS AROUND C1 AND C2 OUT TO 1.61 A *****     STER 200
    1   102  155501          2         1         0      1.0             STER 210
***** FIND COVALENT BONDS SET UP BOND ANGLES AROUND CARBONS *****      STER 220
    1   201                                                             STER 230
***** INITIALIZE MECHANICAL PLOTTER PACKAGE, 203 FOR CPT PACKAGE ***** STER 240
    1   301       11.       11.       30.       1.5                     STER 250
***** 11X11 BOUNDARY, [illegible] 1.5 MARGIN, VIEW FROM 30 INCHES ***** STER 260
    1   501                                                             STER 270
***** ELIMINATE ALL ORIENTING *****                                     STER 280
    1   502  555501          5         1         0      3.2             STER 290
***** INCLUDED SPHERE OF RADIUS 3.2 A ABOUT DUMMY ATOM 5,555,01 *****  STER 300
    5   501  555501    255501    155501    355501    455502            STER 310
***** ORIGIN AT DUMMY ATOM 555501, VIEWING ALONG 3 FOLD AXIS OF CUBANE STER 320
    3   502          2       75.         1       20.                    STER 330
***** ROTATE 75 DEGREES ABOUT Y, THEN 20 DEGREES ABOUT NEW X *****     STER 340
    1   604          0         0         0      1.40                    STER 350
***** AUTOMATIC SCALE AND POSITION, 50 PERCENT PROBABILITY ELLIPSOIDS *STER 360
    2   502          2       3.7                                        STER 370
***** STEREO ROTATION OF 3.7 DEGREES ABOUT Y FOR LEFT EYE *****        STER 380
    1  1101                                                             STER 390
***** START SAVE SEQUENCE *****                                         STER 400
    2   511          0                                                  STER 410
    3         1  0  1  0  0    0.0    1.6   .04                         STER 420
***** STORE PROJECTED ATOMS AND BONDS FOR OVERLAP, REMOVE SET BY OVERLAPSTER 430
    1   715          0         0         1         0       .10       .60       .70STER 440
    1                                    1         2                    STER 450
***** DRAW CARBON ATOM ELLIPSOIDS, ATOM NUMBERS ARE 1-2 *****          STER 460
    1   712                                                  .30       .15       .0STER 470
    1                                    3         4                    STER 480
***** DRAW HYDROGEN ATOM SPHERES, ATOM NUMBERS ARE 3-4 *****           STER 490
    2   812                                                             STER 500
    3         1  0  1  0  0    0.0    1.6   .04                         STER 510
***** TYPE 1 BONDS .04 A [illegible], ATOMS 1-4 TO ATOMS 1-4, 0.0-1.6 A STER 520
    1   906  155504    155503          0         0       .15         0       -.0STER 530
***** LABEL BOND 155504-155503 WITH PARALLEL BOND DISTANCE LABEL *****  STER 540
    1   916  255504    155501          0         0       .15         0       -.0STER 550
***** LABEL BOND 255504-155501 WITH PERPENDICULAR BOND DISTANCE LABEL *STER 560
    3   902  555501          5         5       1.0       .65         0  STER 570
                            CUBANE                                      STER 580
    1  1102                                                             STER 590
***** END OF SAVE SEQUENCE *****                                        STER 600
    1   202       9.                                                    STER 610
***** ADVANCE PLOTTER 9 INCHES ALONG X *****                            STER 620
    1   502          2      -3.7                                        STER 630
***** STEREO ROTATION OF -3.7 DEGREES ABOUT Y FOR RIGHT EYE VIEW ***** STER 640
    1  1103                                                             STER 650
***** EXECUTE SAVED SEQUENCE FOR RIGHT EYE DRAWING *****                STER 660
    1   202      10.                                                    STER 670
***** ADVANCE PLOTTER 10 INCHES *****                                   STER 680
    1   203                                                             STER 690
***** END DUMMY PLOT TO MAGNETIC TAPE *****                             STER 700
       -1                                                               STER 710
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